Computational Studies on High Temperature Superconductivity

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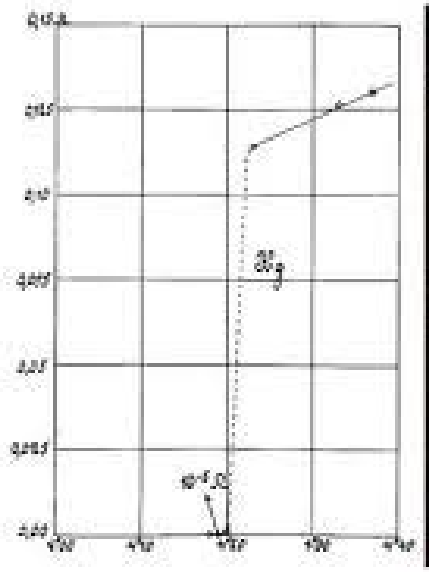
What is superconductivity ?

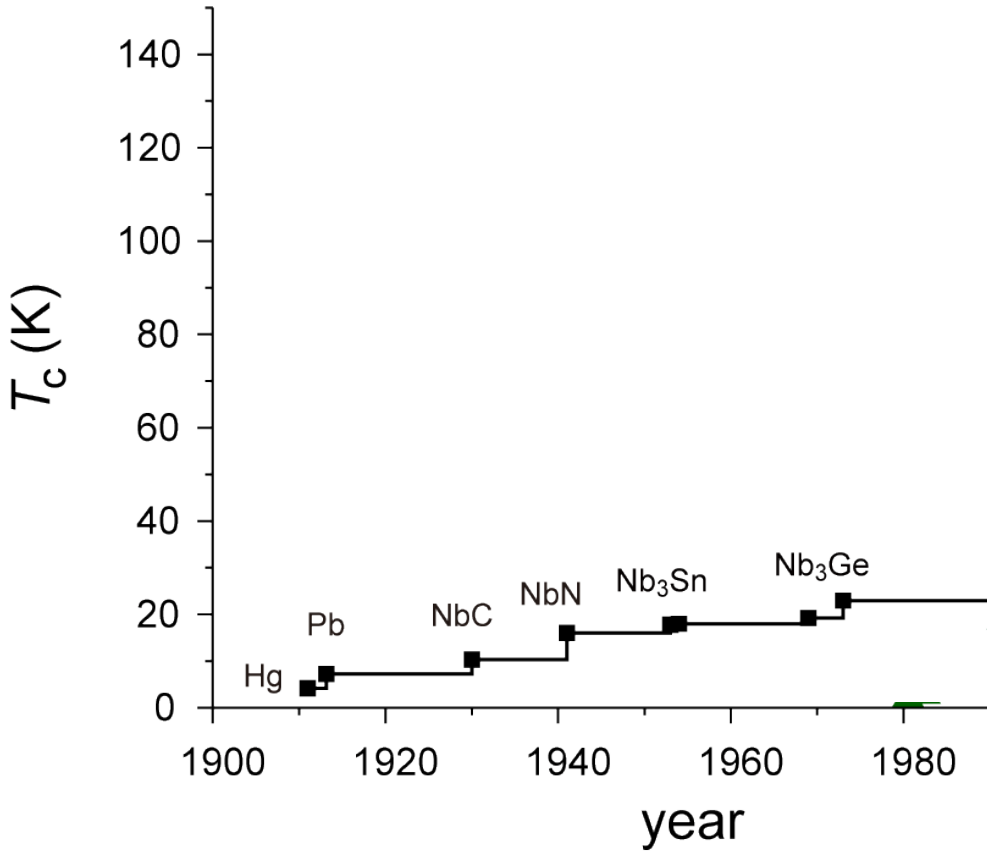


Disappearance of resistivity below
a certain temperature T_c :
superconducting transition temperature

First discovered by Kamerlingh Onnes
In Mercury in 1911
this year 2011 marks the 1st centennial of the discovery of superconductivity

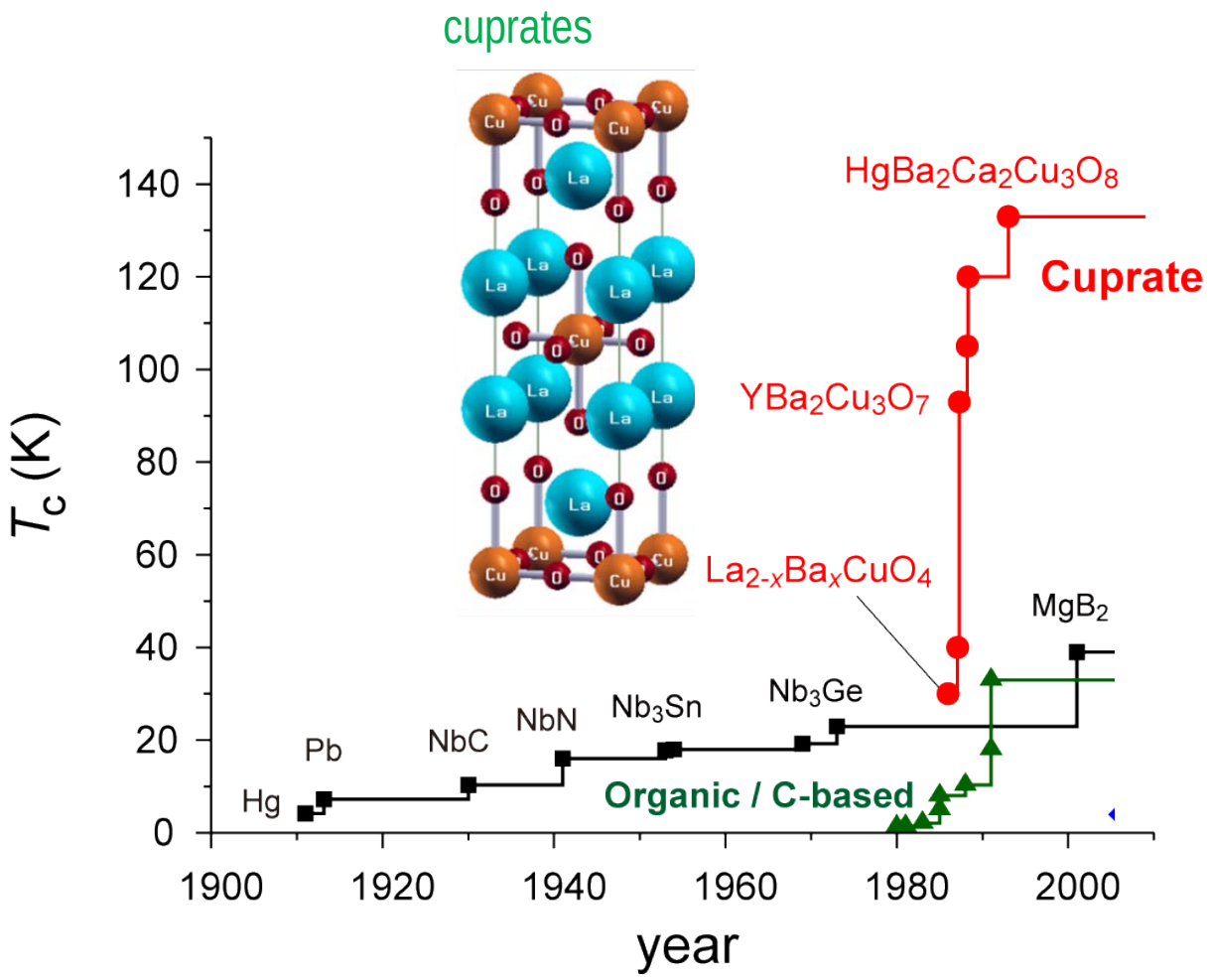
Superconductivity occurs at very low temperature

History of the highest Tc



http://sakaki.issp.u-tokyo.ac.jp/user/kittaka/contents/others/tc-history.html

Discovery of “high Tc” superconductivity



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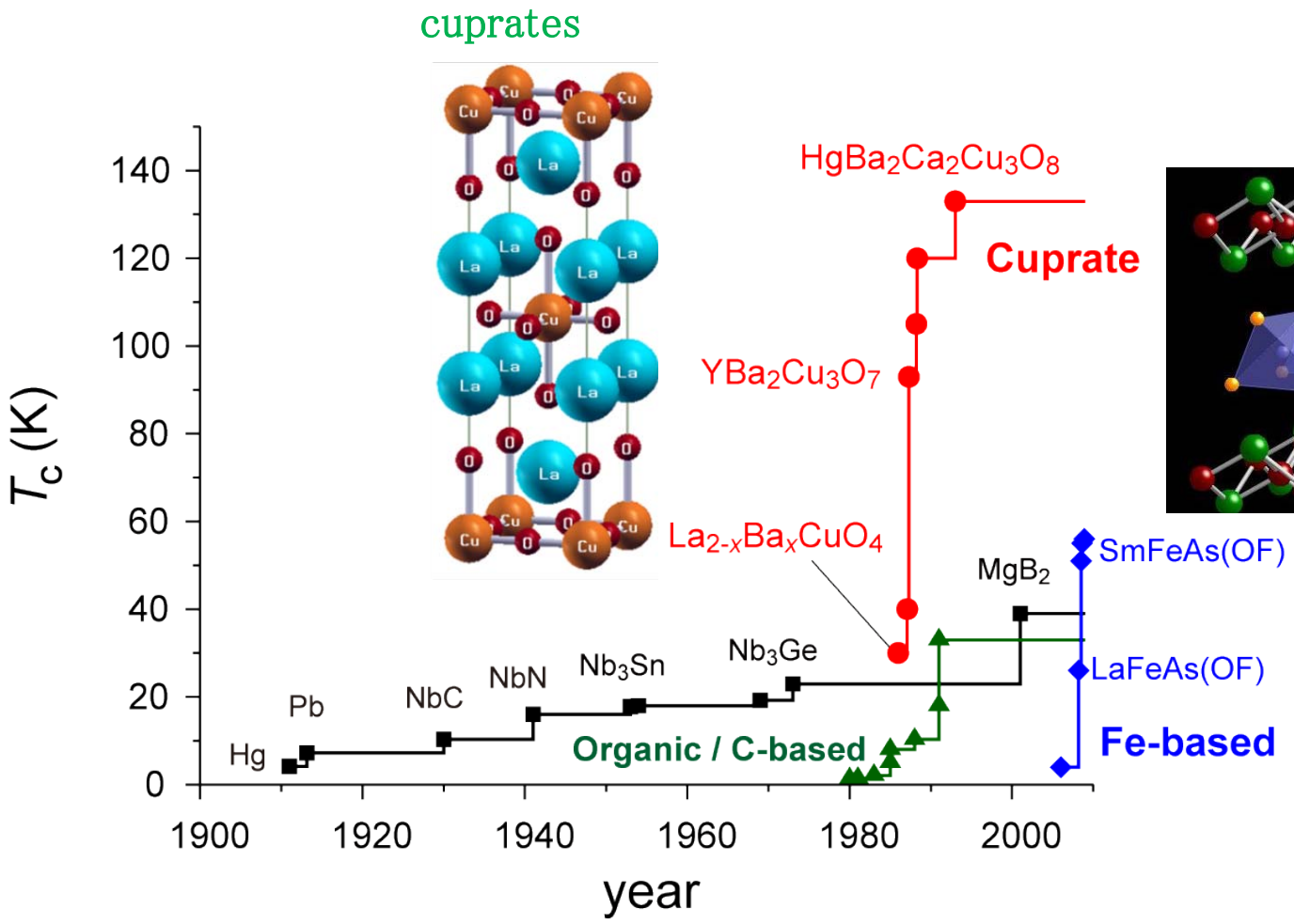
Discovery of “high Tc” superconductivity



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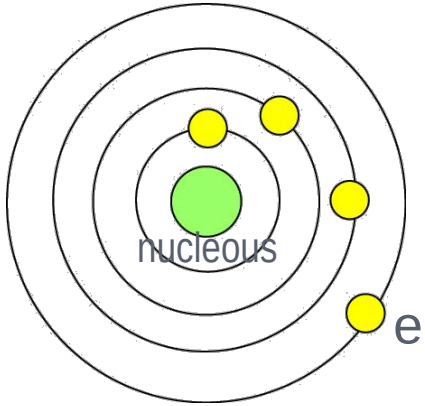
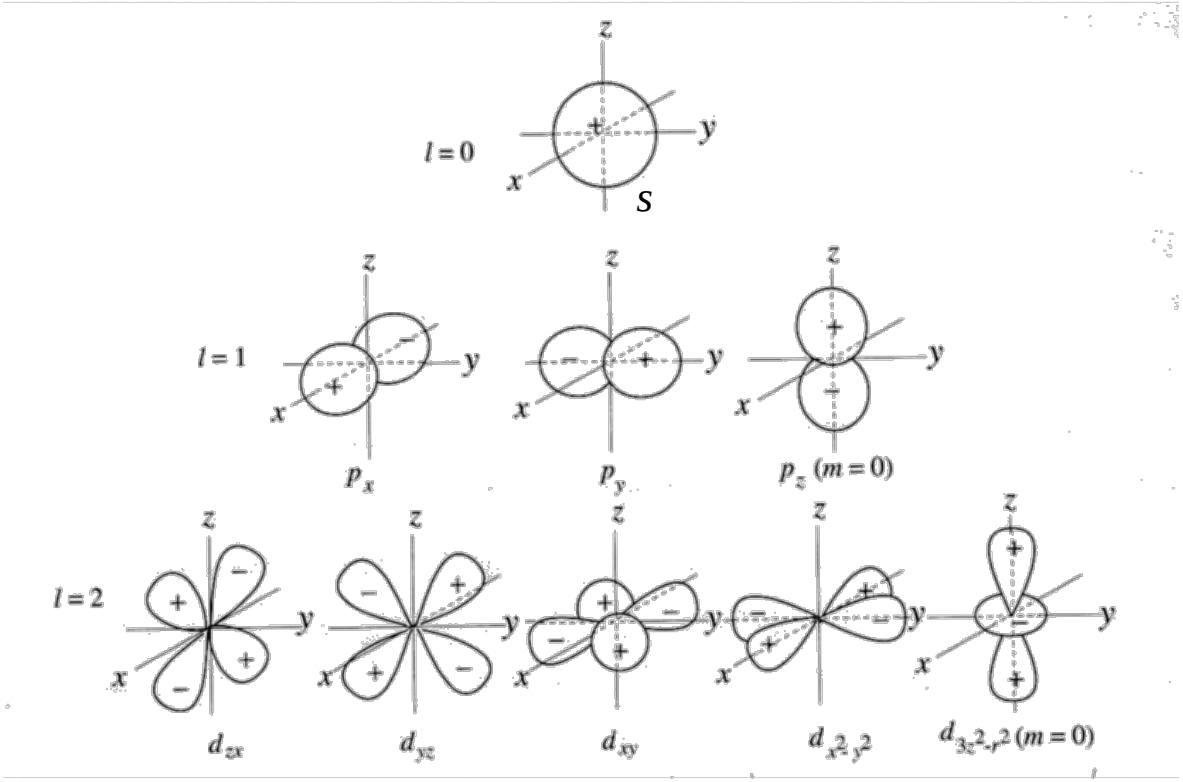
Atoms

atom

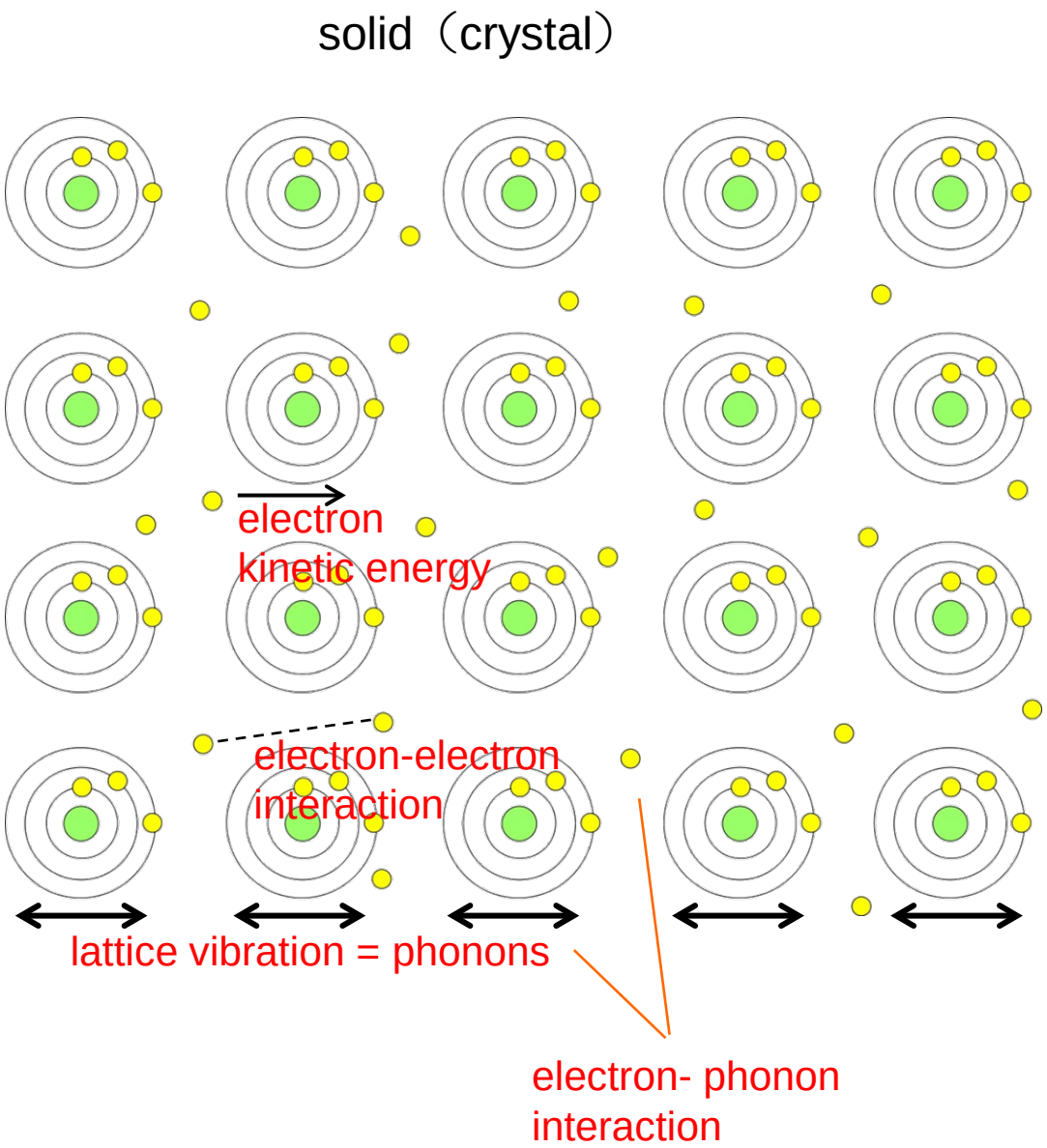


atomic orbitals

orbitals



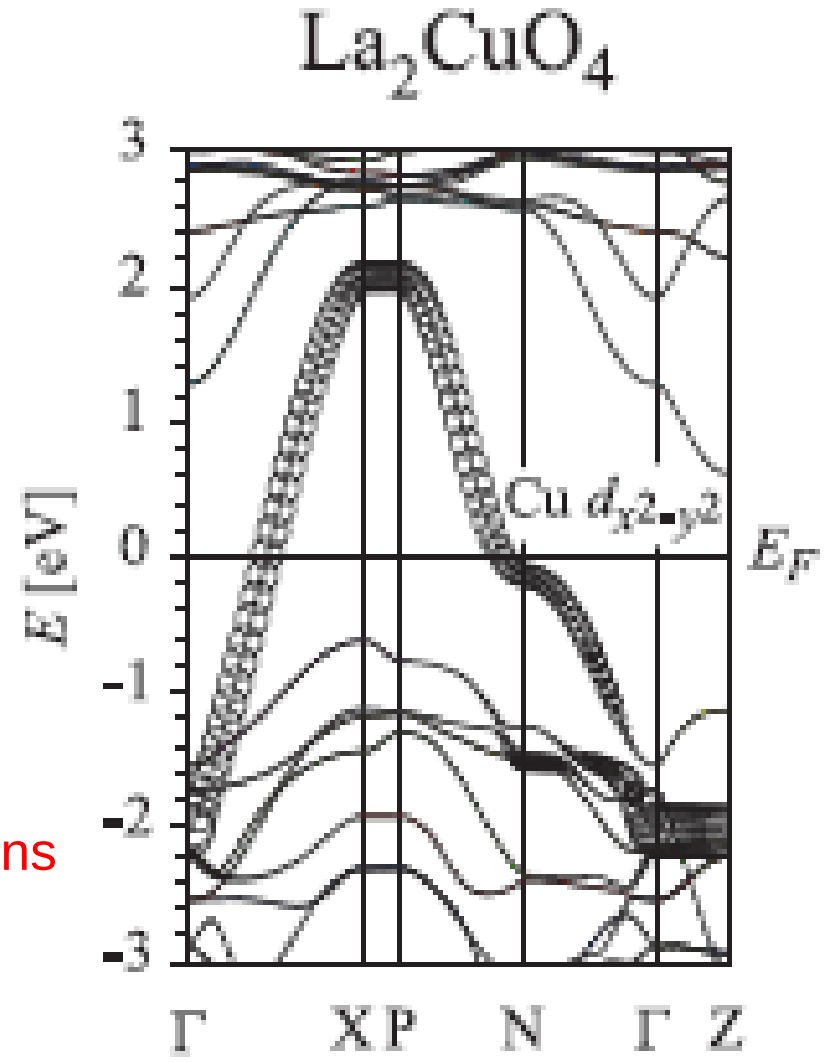
Solids


solid（crystal）
electron
kinetic energy
electron-electron
interaction
lattice vibration = phonons
electron- phonon
interaction

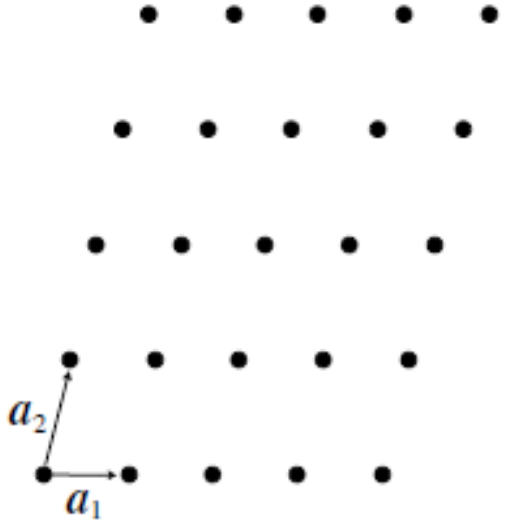
Necessity of Model Hamiltonian

kinetic energy of electrons
=complicated band structure

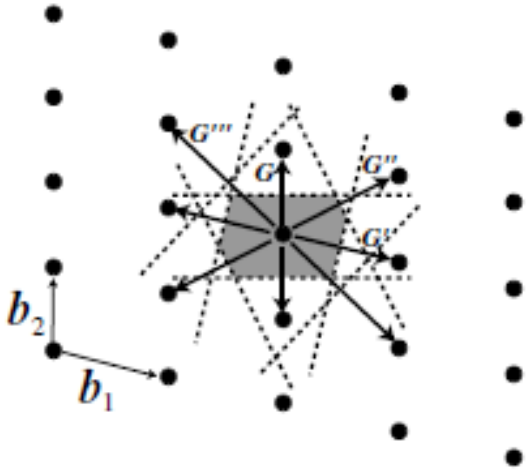
Model Hamiltonian :
consider only essential bands near the Fermi level,
also
simplify the electron-electron and/or electron-phonon interactions



real space lattice



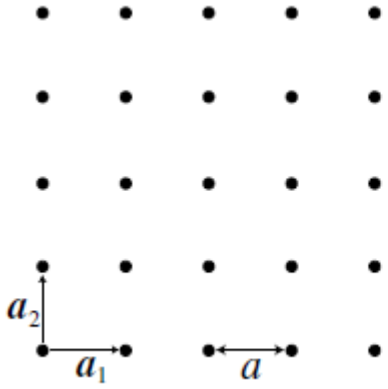
reciprocal lattice
momentum space



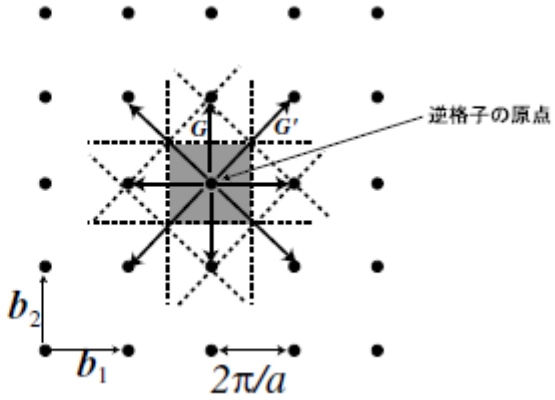
wave number : $k=2\pi/\lambda$

$$\boldsymbol{p=\hbar k}$$

square lattice

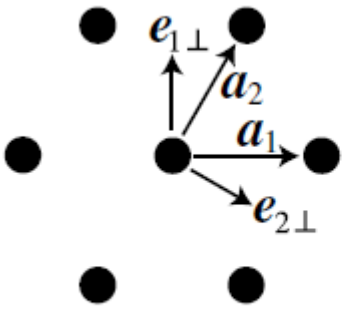


real space

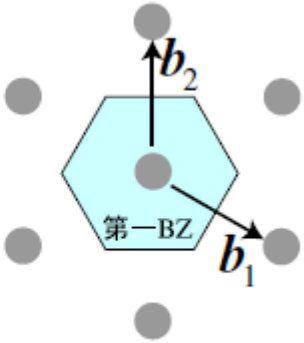


reciprocal space

triangular lattice



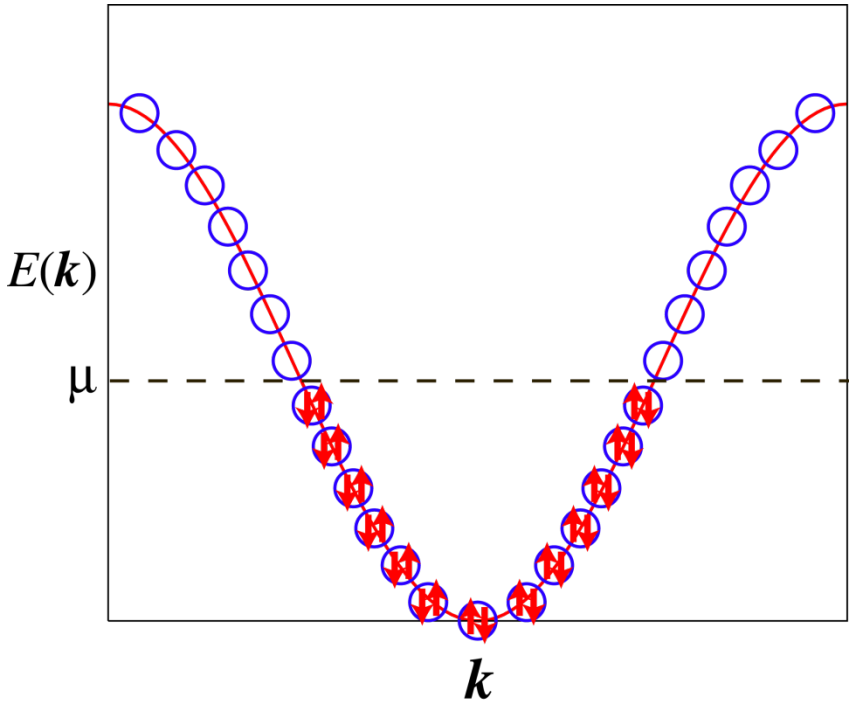
real space



reciprocal space

Energy band, Fermi sea, Fermi surface

Electrons : Fermions →In the ground state (T=0),
the electrons are filled from the bottom of the band up to the Fermi energy.



μ, E_F : Fermi energy, chemical potential

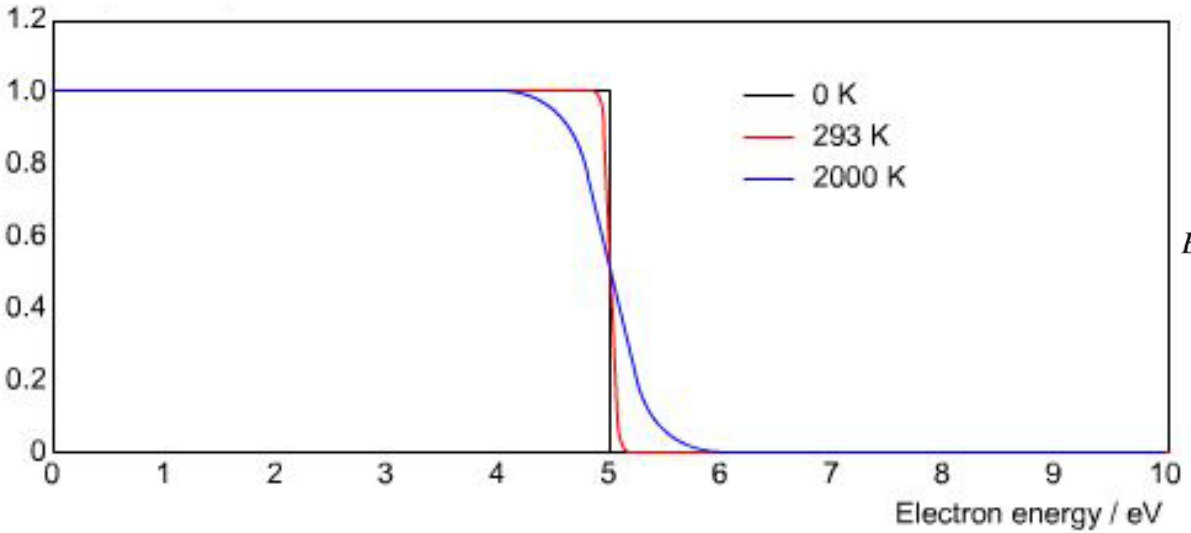
constant energy surface with $E(k) = E_F$:

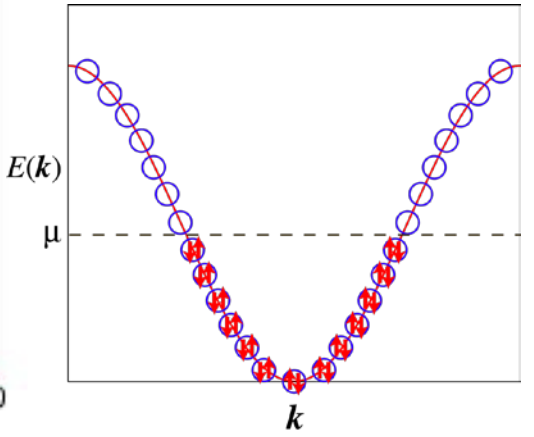
Fermi surface of free electron gas is a sphere

Fermi distribution function

$$f(\varepsilon) = \frac{1}{\exp(\frac{\varepsilon-\mu}{k_B T})+1}$$

average number of electrons occuping
a single state with energy ε at temperature *T*

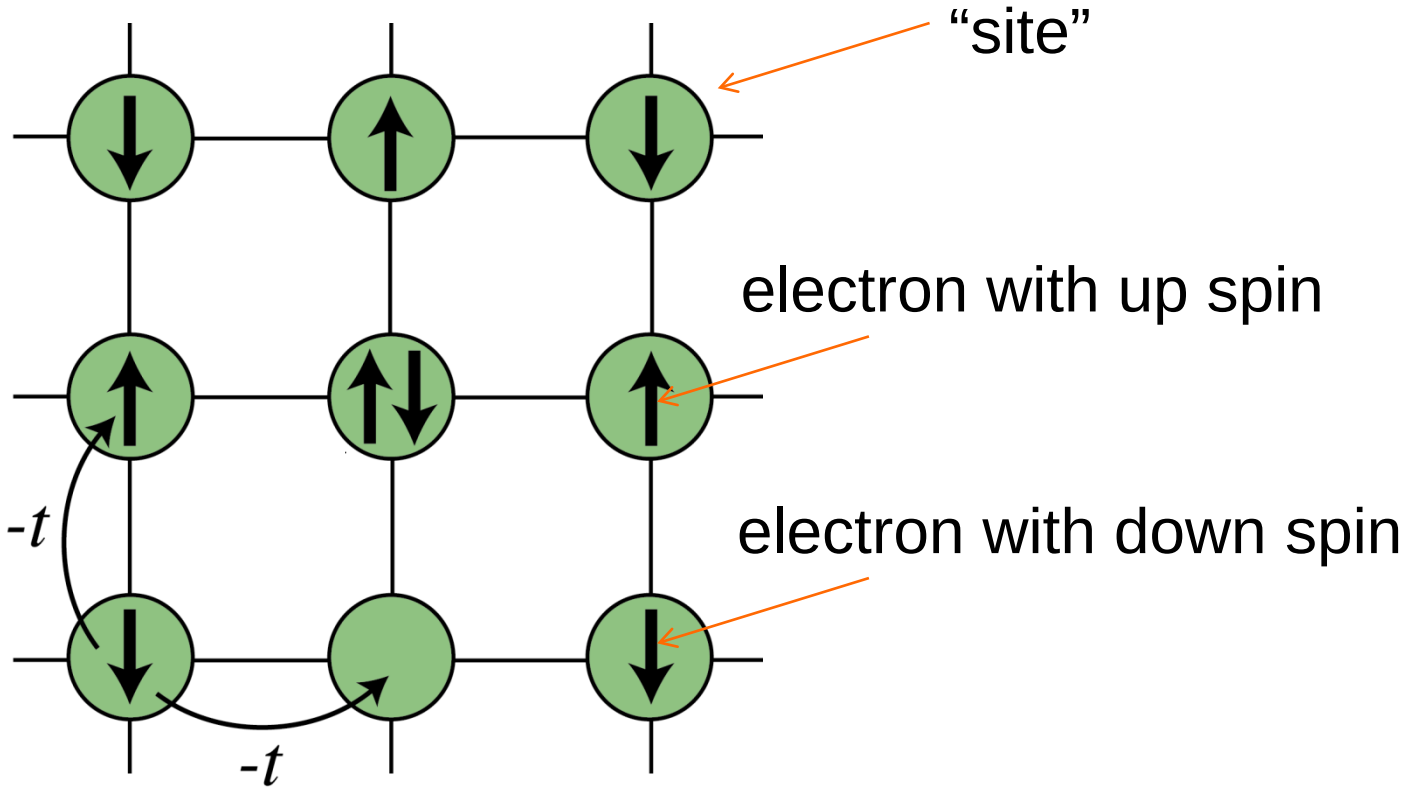




Tightbinding models

In 1D

In 2D



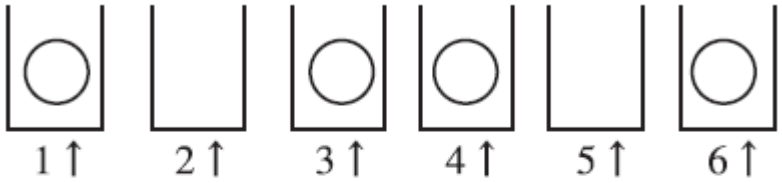
“hopping integral”

creation, annihilation operators in real space

number representation

$$c_{i\sigma}^{\dagger}|\cdots,0,\cdots\rangle_{\sigma}=|\cdots,1,\cdots\rangle_{\sigma}$$

$$c_{i\sigma}|\cdots,1,\cdots\rangle_{\sigma}=|\cdots,0,\cdots\rangle_{\sigma}$$



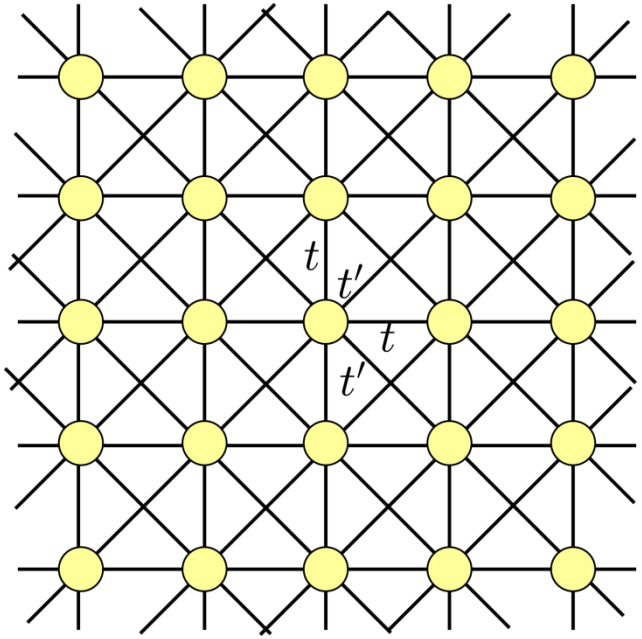
$$|\,1,0,1,1,0,1\rangle_{\uparrow} = c_{1\uparrow}^{\dagger}\,c_{3\uparrow}^{\dagger}\,c_{4\uparrow}^{\dagger}\,c_{6\uparrow}^{\dagger}|0\rangle$$

anticommutation relation of Fermion operators

$$\{c_{i\sigma},c_{j\sigma'}\}=\{c_{i\sigma}^{\dagger},c_{j\sigma'}^{\dagger}\}=0,\qquad \{c_{i\sigma},c_{j\sigma'}^{\dagger}\}=\delta_{ij}\delta_{\sigma\sigma'}$$

$$\{A,B\}=AB+BA$$

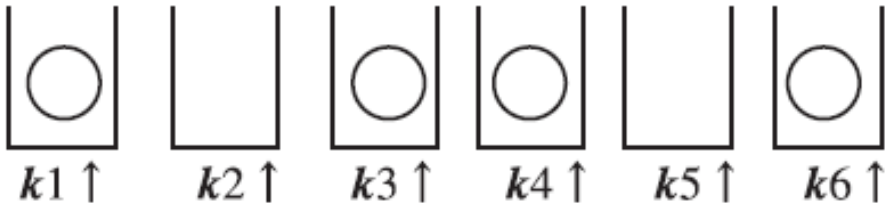
Tight binding model expressed in second quantization form



$$H = \sum_{ij} \sum_{\sigma} t(\boldsymbol{R}_i - \boldsymbol{R}_j) c^{\dagger}_{i\sigma} c_{j\sigma}$$

creation, annihilation operators in momentum space

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} c_{\boldsymbol{k}\sigma}$$



the number of k's
=the number o sites
(# of unit cells)

$$= \left| 1,0,1,1,0,1 \right\rangle_{\uparrow} = c^{\dagger}_{k1\uparrow} c^{\dagger}_{k3\uparrow} c^{\dagger}_{k4\uparrow} c^{\dagger}_{k6\uparrow} \left| 0 \right\rangle$$

$$H = \sum_{\boldsymbol{k},\sigma} \varepsilon(\boldsymbol{k}) c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$$

"diagonal" ;
number operator in
momentum space

$$\varepsilon(\boldsymbol{k}) = \varepsilon(-\boldsymbol{k}) = \sum_{\boldsymbol{r}} \exp(-i\boldsymbol{k}\cdot\boldsymbol{r}) t(\boldsymbol{r})$$

band dispersion

Grand partition function and Fermi's distribution function

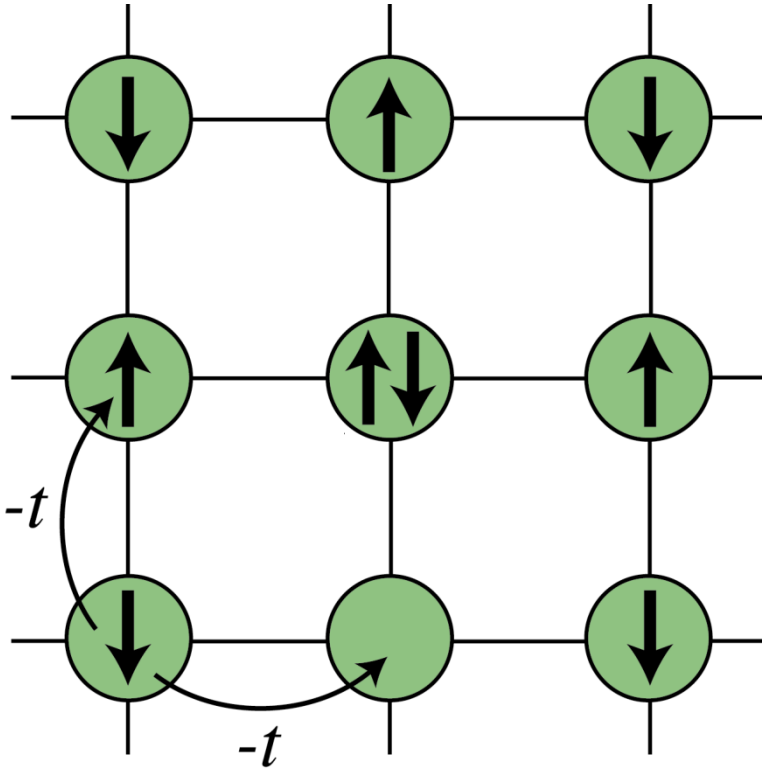
$$\Xi = \mathrm{Tr}\ \exp\{-\beta(H-\mu N)\} \qquad \beta = \frac{1}{k_B T}$$

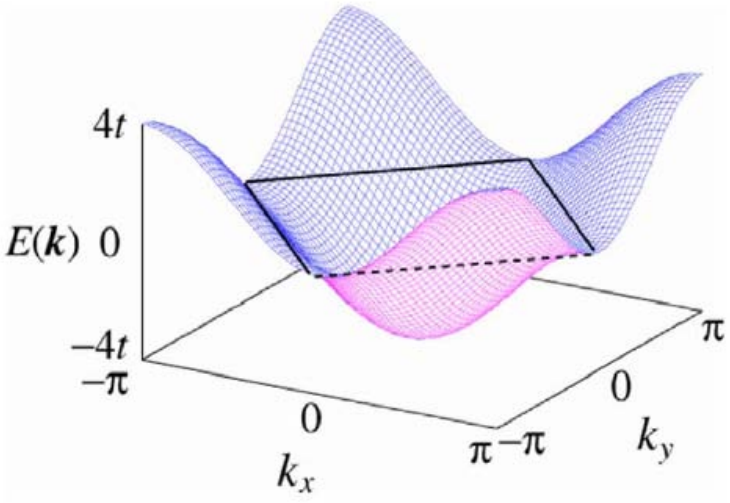
$$H-\mu N = \sum_{k,\sigma} \varepsilon(k) c^{\dagger}_{k\sigma} c_{k\sigma} - \mu \sum_{k,\sigma} c^{\dagger}_{k\sigma} c_{k\sigma}$$

$$= \sum_{k,\sigma} \underbrace{\{\varepsilon(k)-\mu\}}_{\| \ \xi(k)} c^{\dagger}_{k\sigma} c_{k\sigma}$$

$$\langle n_{k\sigma} \rangle = \frac{\mathrm{Tr} c^{\dagger}_{k\sigma} c_{k\sigma} \exp\{-\beta(H-\mu N)\}}{\Xi} = \frac{1}{\exp\{\beta\xi(k)\}+1}$$

Tight binding model on a square lattice



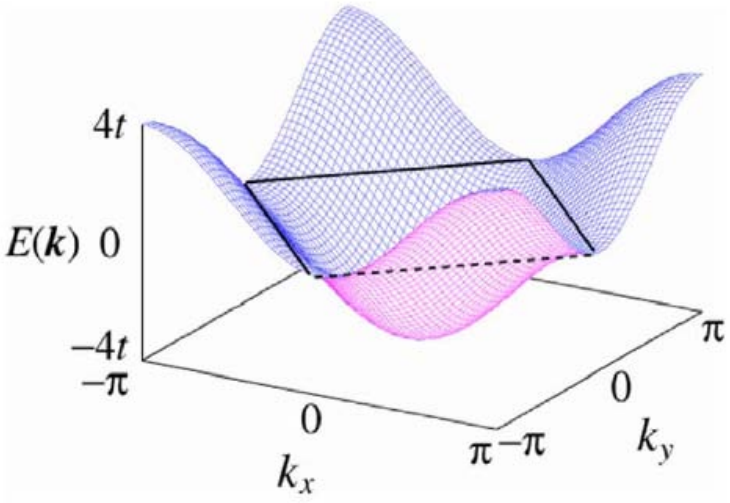


when only the nearest neighbor hopping is considered :

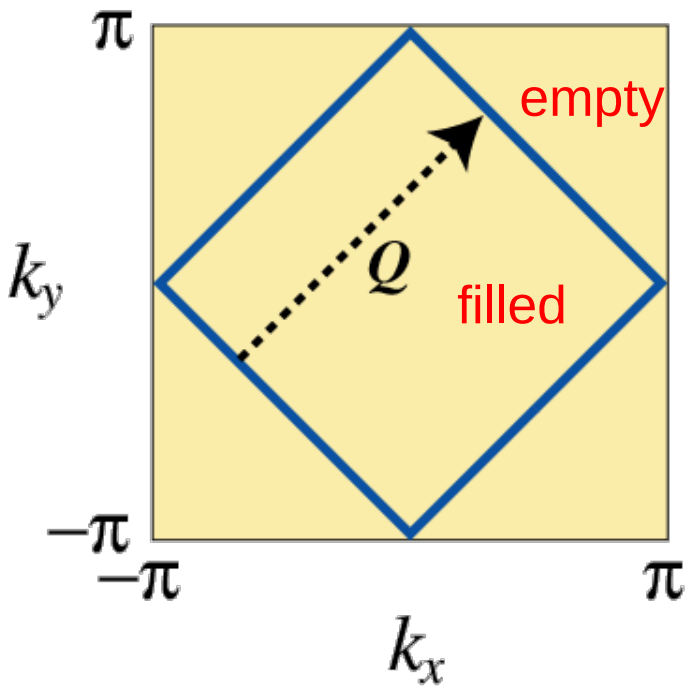
$$\varepsilon(k_x, k_y) = \frac{1}{N} N(-t)[\exp(ik_x a) + \exp(ik_y a) + \exp(-ik_x a) + \exp(-ik_y a)] = -2t[\cos(k_x a) + \cos(k_y a)]$$

When there are *M* sites in a unit cell, and each site contains *L* orbitals, it is a *ML* band model

Fermi surface



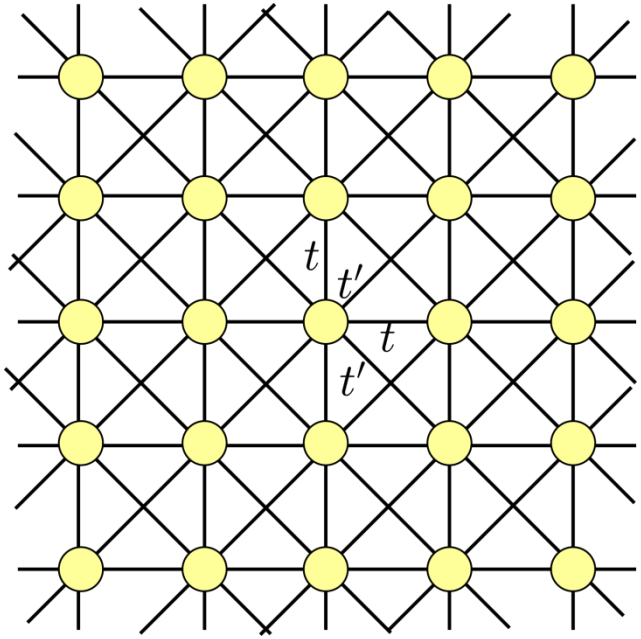
Fermi surface at half-filling

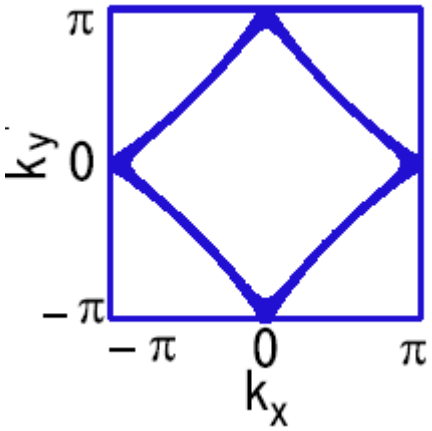


Fermi surface is “well nested” when it has a large overlap with the one translated by a certain “nesting vector Q”

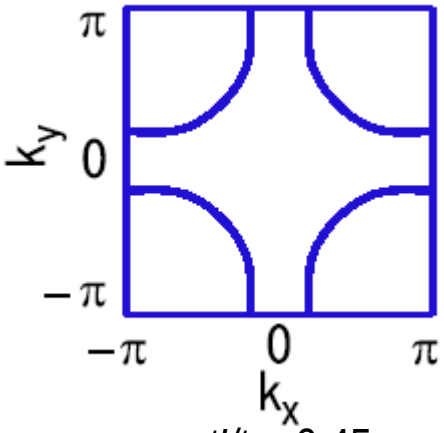
Effect of distant hoppings

Fermi surface for band filling n=0.85

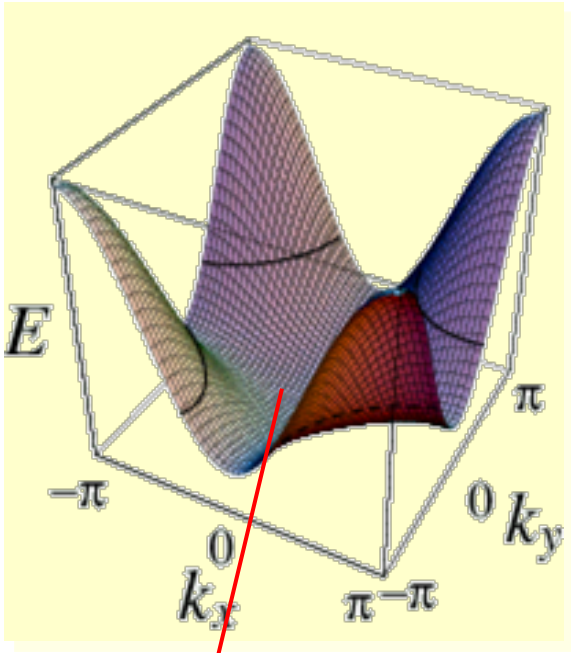




t'/t =-0.2



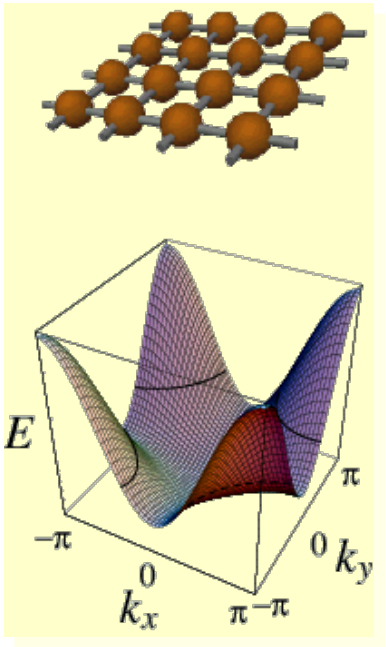
t'/t =-0.45



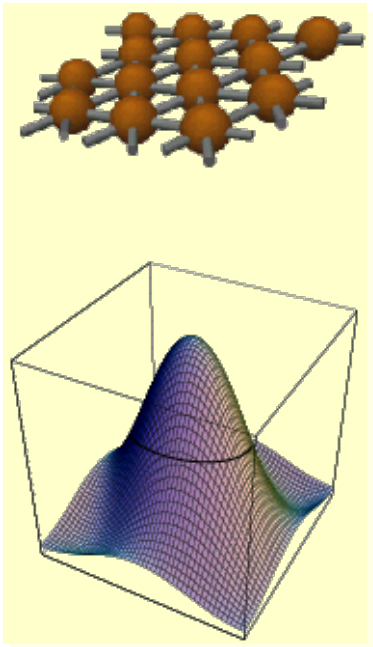
flattening of the band

Tightbinding model band dispersion on various lattices

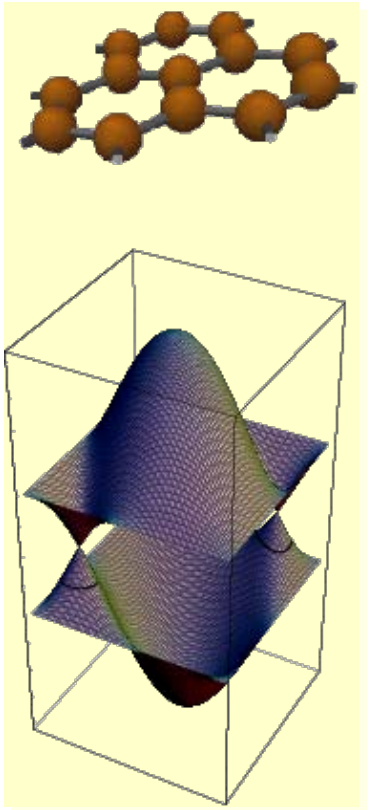
square lattice



triangular



honeycomb



Introduction of electron-electron interaction

number operator

$$n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$$

$$n_{i\sigma} \left| \cdots, n, \cdots \right\rangle_{\uparrow} = n \left| \cdots, n, \cdots \right\rangle_{\sigma}, \qquad (n = 0 \quad \text{or} \quad 1)$$

Hamiltonian in real space

$$H = \sum_{ij} \sum_{\sigma} t(\boldsymbol{R}_i - \boldsymbol{R}_j) c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{ij} \sum_{\sigma\sigma'} v(\boldsymbol{R}_i - \boldsymbol{R}_j) n_{i\sigma} n_{j\sigma'}$$

Hamiltonian in momentum space

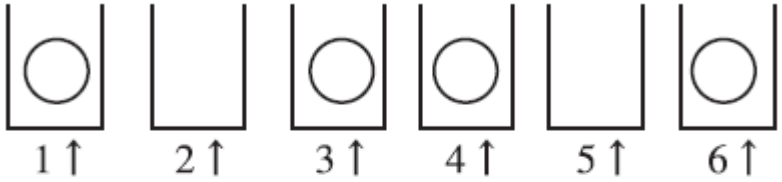
$$H = \sum_{\boldsymbol{k},\sigma} \varepsilon(\boldsymbol{k}) c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \frac{1}{2} \sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}} \sum_{\sigma\sigma'} V(\boldsymbol{q}) c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}\sigma} c^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q}\sigma'} c_{\boldsymbol{k}'\sigma'} c_{\boldsymbol{k}\sigma}$$

$$\varepsilon(\boldsymbol{k}) = \varepsilon(-\boldsymbol{k}) = \sum_{\boldsymbol{r}} \exp(-i\boldsymbol{k} \cdot \boldsymbol{r}) t(\boldsymbol{r})$$

$$V(\boldsymbol{q}) = V(-\boldsymbol{q}) = \frac{1}{N} \sum_{\boldsymbol{r}} \exp(-i\boldsymbol{q} \cdot \boldsymbol{r}) v(\boldsymbol{r})$$

Difficulty in solving a many body problem

most straight forward way : exact diagonalization of the Hamiltonian matrix



basis to obtain H matrix :

$$|\,1,0,1,1,0,1\rangle_{\uparrow} = c^{\dagger}_{1\uparrow} c^{\dagger}_{3\uparrow} c^{\dagger}_{4\uparrow} c^{\dagger}_{6\uparrow} |0\rangle$$

For instance, for a 20 site system with 10 up spin and 10 down spin electrons, the number of basis is

$({}_{20}C_{10})^2 \sim 3 \times 10^{10}$

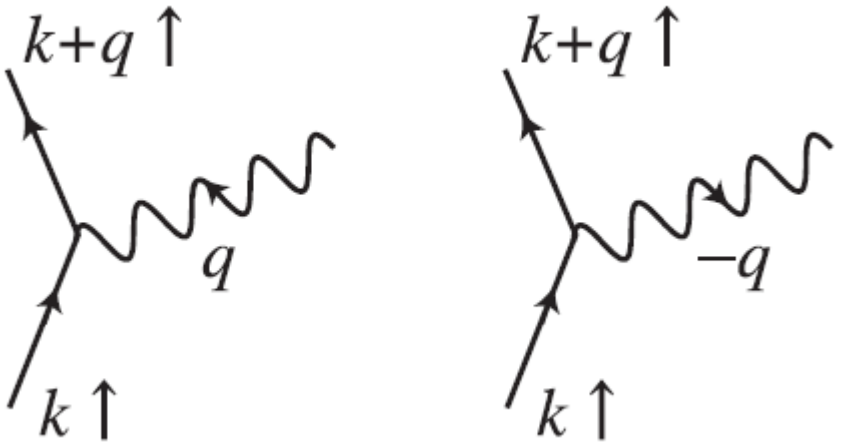
diagonalization of $\sim 10^{10} \times 10^{10}$ matrix is necessary !

(for *only* 20 sites<< 10^{23})

Theory of conventional superconductivity : phonon-mediated pairing and BCS theory

electron-phonon interaction

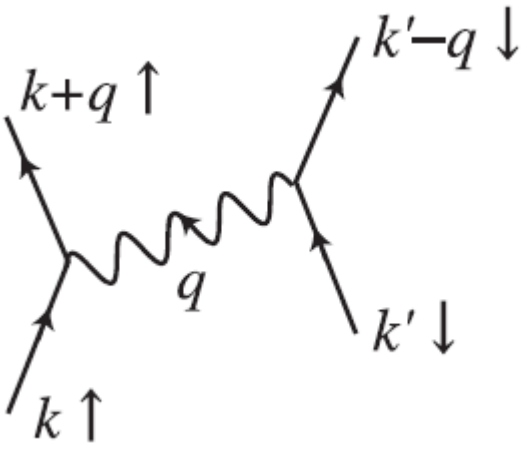
$$H_{\mathrm{el-ph}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q},\sigma} \alpha(\mathbf{q})(a_{\mathbf{q}} + a^{\dagger}_{-\mathbf{q}}) c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma}$$



“Feynman diagrams”

electron-electron effective interaction mediated by phonons

$$H_{\text{eff}} = -\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}\sigma,\sigma} \frac{\alpha^2(\mathbf{q})}{\hbar\omega(\mathbf{q})} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}$$



extract the interaction of the form

$$(\mathbf{k}\uparrow, -\mathbf{k}\downarrow) \rightarrow (\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow)$$

$$H = \sum_{\boldsymbol{k},\sigma} \xi(\boldsymbol{k}) c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k}'} V(\boldsymbol{k}-\boldsymbol{k}') c^\dagger_{-\boldsymbol{k}'\downarrow} c^\dagger_{\boldsymbol{k}'\uparrow} c_{\boldsymbol{k}\uparrow} c_{-\boldsymbol{k}\downarrow}$$

rewrite H-μN as H

V is called the pairing interaction

mean field approximation

$SS \longrightarrow$

$\langle S\rangle\ S + S\ \langle S\rangle$
$- \langle S\rangle\langle S\rangle$

$CCCC \longrightarrow$

$\langle CC\rangle CC + CC\langle CC\rangle$
$- \langle CC\rangle\langle CC\rangle$

Then the Hamiltonian is approximated as

$$\mathcal{H}_{\rm BCS} = \sum_{\mathbf{k}\sigma} \xi(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \Delta(\mathbf{k}) \left(c^\dagger_{-\mathbf{k}\downarrow} c^\dagger_{\mathbf{k}\uparrow} + \text{H.c} \right)$$
$$+ \sum_{\mathbf{k}} \Delta(\mathbf{k}) \langle c^\dagger_{-\mathbf{k}\downarrow} c^\dagger_{\mathbf{k}\uparrow} \rangle$$

not diagonal

where

$$\Delta(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} V(\boldsymbol{k} - \boldsymbol{k}') \langle c_{\boldsymbol{k}'\uparrow} c_{-\boldsymbol{k}'\downarrow} \rangle$$

“order parameter”, “gap function”

Bogoliubov transformation :

creation, annhilation operators of “quasiparticles”

$$\begin{aligned} \alpha_{\mathbf{k}\uparrow} &= u_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\downarrow} \\ \alpha_{-\mathbf{k}\downarrow} &= u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} + v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} \end{aligned}$$

$$\begin{aligned} c_{\mathbf{k}\uparrow} &= u_{\mathbf{k}} \alpha_{\mathbf{k}\uparrow} + v_{\mathbf{k}} \alpha^{\dagger}_{-\mathbf{k}\downarrow} \\ c_{-\mathbf{k}\downarrow} &= u_{\mathbf{k}} \alpha_{-\mathbf{k}\downarrow} - v_{\mathbf{k}} \alpha^{\dagger}_{\mathbf{k}\uparrow} \end{aligned}$$

$$u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$$

required for anticommutation relation

Expressing the Hamiltonian in terms of α, $\alpha\dagger$ and enforcing

$$2\xi(\mathbf{k}) u_{\mathbf{k}} v_{\mathbf{k}} + \Delta(\mathbf{k}) v_{\mathbf{k}}^2 - \Delta(\mathbf{k}) u_{\mathbf{k}}^2 = 0$$

$$\mathcal{H} = E_{\mathrm{GS}} + \sum_{\mathbf{k}} E(\mathbf{k})(\alpha^{\dagger}_{\mathbf{k}\uparrow}\alpha_{\mathbf{k}\uparrow} + \alpha^{\dagger}_{-\mathbf{k}\downarrow}\alpha_{-\mathbf{k}\downarrow}),$$

$$E_{\mathrm{GS}} = \sum_{\mathbf{k}} \left[2\xi(\mathbf{k})v^2_{\mathbf{k}} + 2\Delta(\mathbf{k})u_{\mathbf{k}}v_{\mathbf{k}} + \Delta(\mathbf{k})\langle c^{\dagger}_{-\mathbf{k}\downarrow}c^{\dagger}_{\mathbf{k}\uparrow}\rangle\right]$$: ground state energy

$$u^2_{\mathbf{k}} = \frac{1}{2}\left[1 + \frac{\xi(\mathbf{k})}{E(\mathbf{k})}\right],$$

$$v^2_{\mathbf{k}} = \frac{1}{2}\left[1 - \frac{\xi(\mathbf{k})}{E(\mathbf{k})}\right],$$

$$E(\mathbf{k}) = \sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}$$

$$|\Psi_{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow}\right)|0\rangle$$: ground state

since the “quasiparticles” are “free particles”

$$\langle \alpha^\dagger_{\mathbf{k}\uparrow} \alpha_{\mathbf{k}\uparrow} \rangle = \langle \alpha^\dagger_{-\mathbf{k}\downarrow} \alpha_{-\mathbf{k}\downarrow} \rangle = f(E(\mathbf{k}))$$

$$f(E) \equiv 1/(e^{\beta E} + 1)$$

this gives

$$\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle = \frac{\Delta(\mathbf{k})}{2E(\mathbf{k})} \tanh\left(\frac{1}{2}\beta E(\mathbf{k})\right)$$

Then, from the definition of Δ

$$\Delta(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} V(\boldsymbol{k}-\boldsymbol{k}') \frac{\Delta(\boldsymbol{k}')}{2E(\boldsymbol{k}')} \tanh\left(\frac{1}{2}\beta E(\boldsymbol{k}')\right)$$

$$E(\boldsymbol{k}) = \sqrt{\xi(\boldsymbol{k})^2 + |\Delta(\boldsymbol{k})|^2}$$

This is an equation that self-consistently determines Δ :

“gap equation”

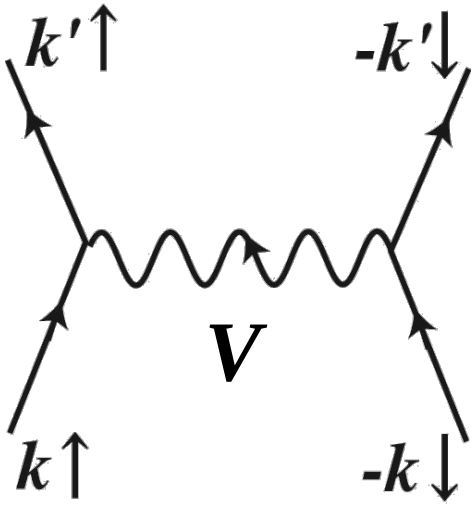
$$E(\boldsymbol{k}) = \sqrt{\xi(\boldsymbol{k})^2 + |\Delta(\boldsymbol{k})|^2}$$

gives the dispersion of the excitation of quasiparticles

→there is a gap around $\xi=0$, the ground state is protected by the gap

superconductivity occurs due to pair scattering

$V(k\text{-}k')$: pairing interaction → pair scattering



gap equation

$$\Delta(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} \frac{\tanh[E(\boldsymbol{k}')/k_B T]}{2E(\boldsymbol{k}')} V\ (\boldsymbol{k}-\boldsymbol{k}')\Delta(\boldsymbol{k}')$$

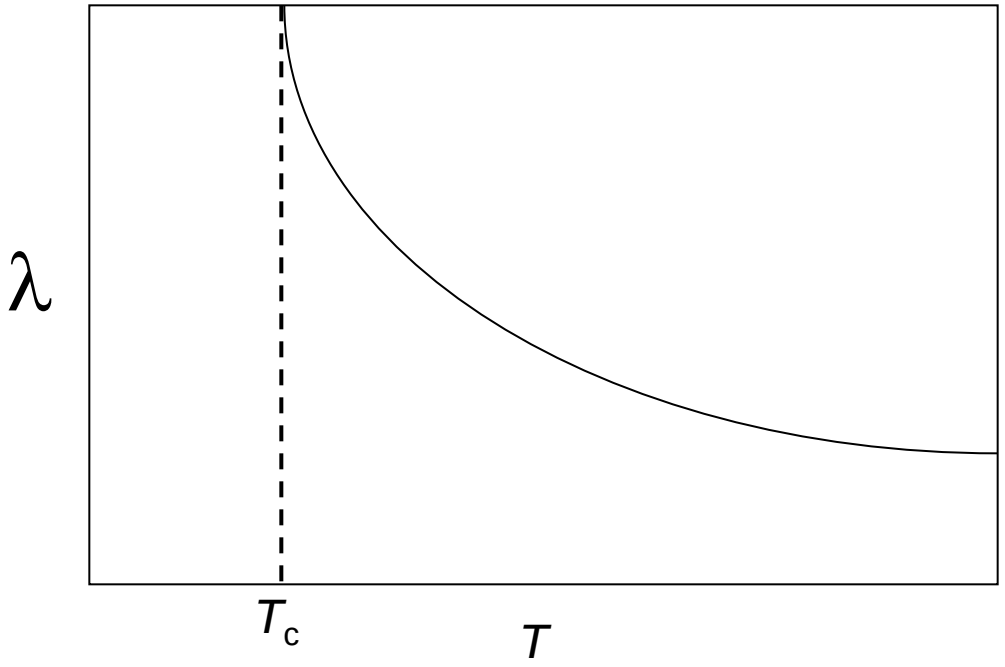
$$E(\boldsymbol{k}) = \sqrt{\xi(\boldsymbol{k})^2 + |\Delta(\boldsymbol{k})|^2}$$

In order to have a finite Δ

$$V\ (\boldsymbol{k}-\boldsymbol{k}')\Delta(\boldsymbol{k})\Delta(\boldsymbol{k}') < 0$$

Linearized gap equation : neglect O(Δ^2) or T$\sim$Tc

$$\lambda\Delta(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} \frac{\tanh[\varepsilon(\boldsymbol{k}')/k_B T]}{2\varepsilon(\boldsymbol{k}')} V(\boldsymbol{k}-\boldsymbol{k}')\Delta(\boldsymbol{k}')$$



if $V(\boldsymbol{q})$=constant,

$$\Delta(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} \frac{\tanh[E(\boldsymbol{k}')/k_B T]}{2E(\boldsymbol{k}')} V \quad (\boldsymbol{k}-\boldsymbol{k}')\Delta(\boldsymbol{k}')$$

shows that Δ is independent of $\boldsymbol{k}$

This means that finite Δ is obtained only when V<0 : attractive interaction

phonon mediated interaction satisfies the condition

$$H_{\text{eff}} = -\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}\sigma,\sigma'} \frac{\alpha^2(\mathbf{q})}{\hbar\,\omega(\mathbf{q})} c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} c^{\dagger}_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}$$

assuming that *V* is small, Tc is approximately given as,

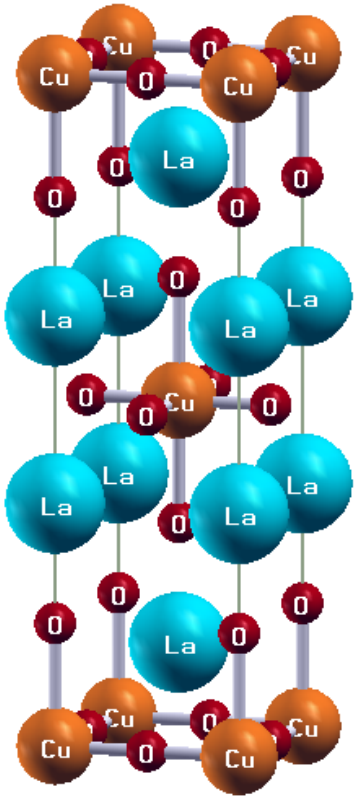
$$k_B T_c = 1.13\,\hbar\omega_D \exp\left(-\frac{1}{VD(\varepsilon_F)}\right)$$

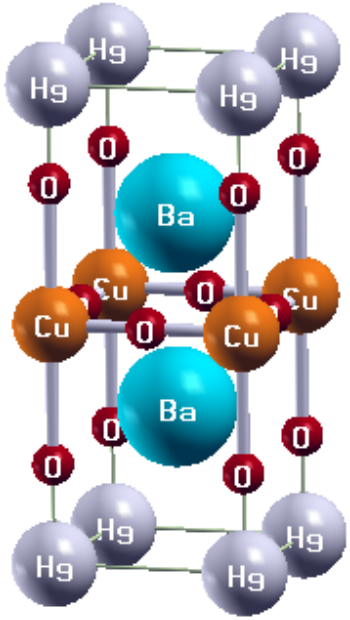
ω_D is the maximum frequency of the phonons,
usually $\hbar\omega_D/k_B$ is O(100K)

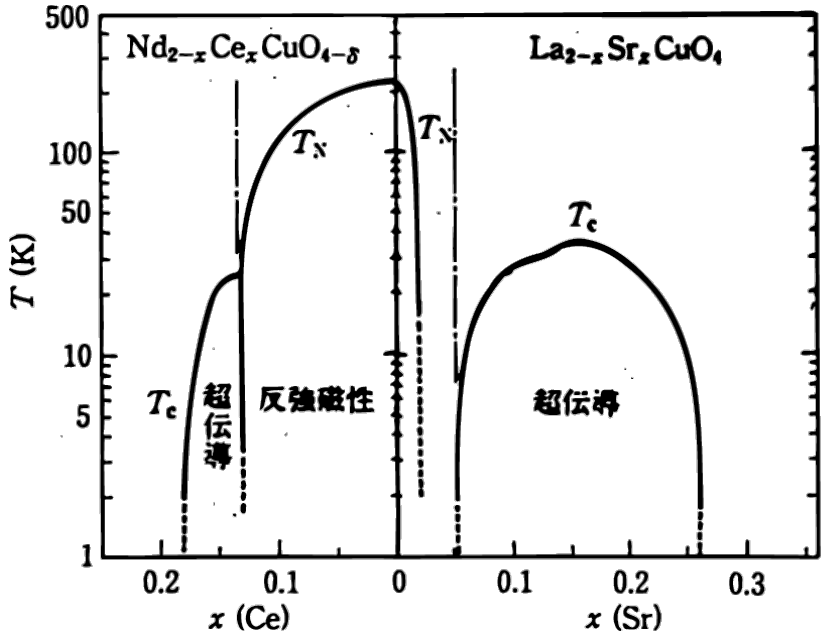
$D(\varepsilon_F)$ is the density of states at the Fermi energy,
usually $VD(\varepsilon_F) \ll 1$

for strong coupling superconductors with $VD(\varepsilon_F) \sim 1$
further analysis have shown that the upper bound for Tc is few 10K

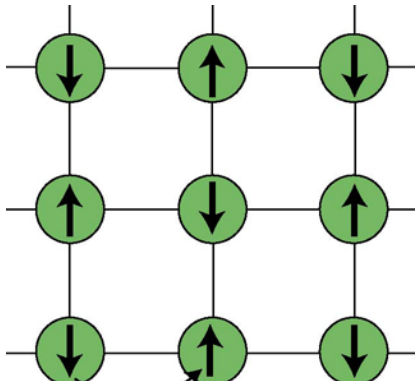
Cuprate high T_c superconductors







antiferromagnetic spin ordering
in the parent, undoped compound



Properties of the cuprates and possibility of unconventional superconductivity

T_c beyond 100K

superconductivity near antiferromagnetism

strong electron correlation

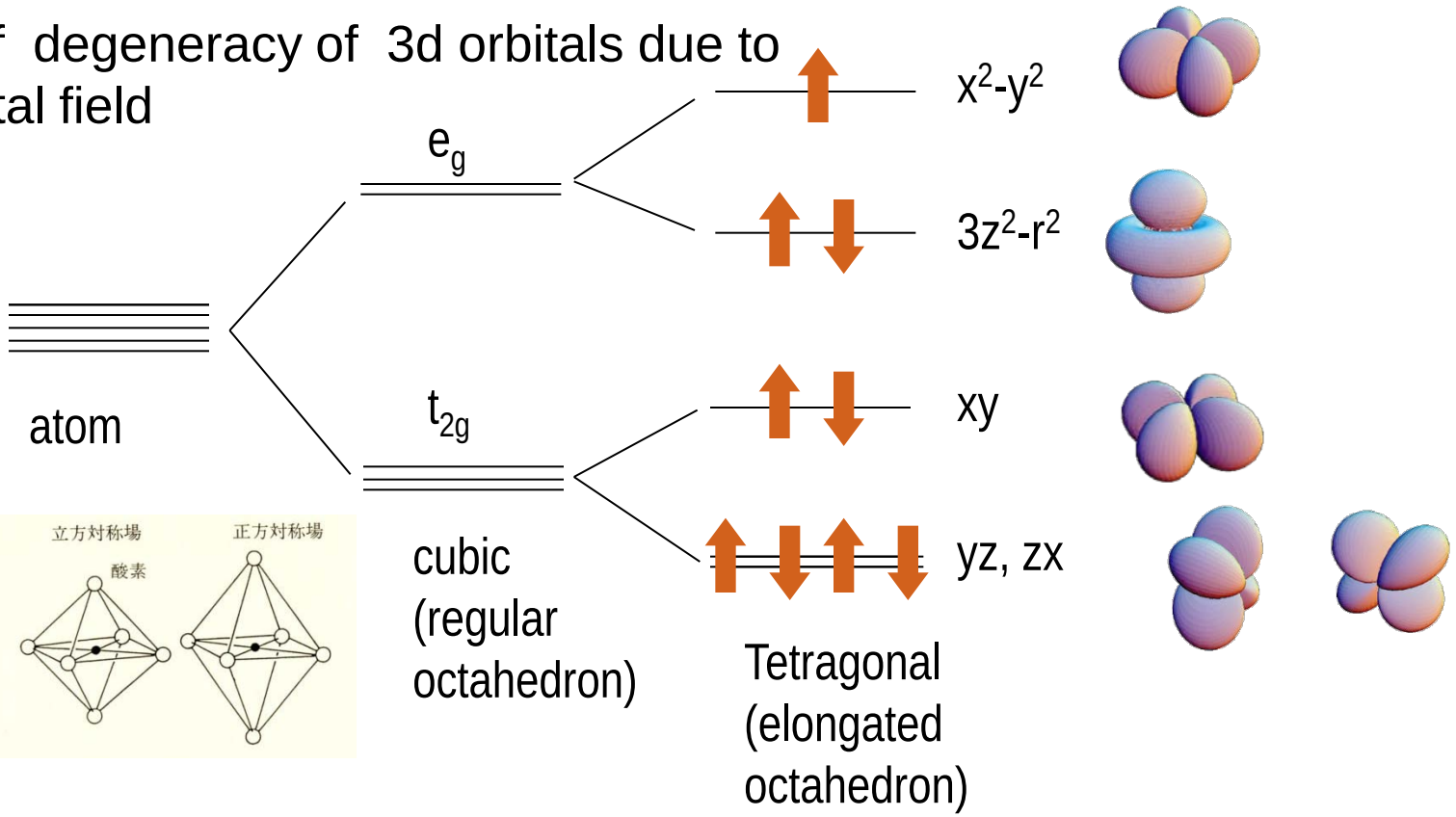
d-wave pairing

→ phonon mediated Cooper pairing is unlikely

→ necessity of *purely electronic* model Hamiltonian

Crystal field effect

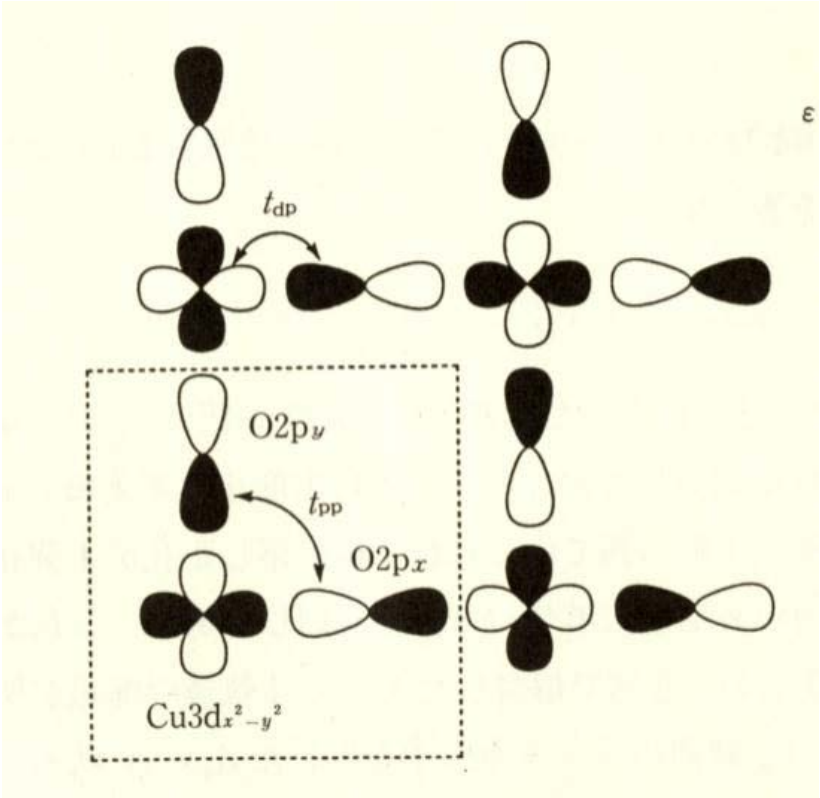
lift of degeneracy of 3d orbitals due to crystal field



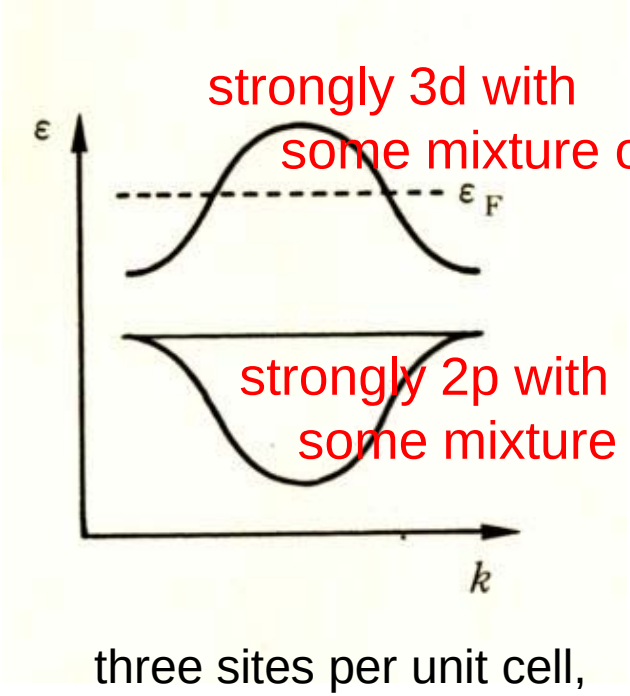
$La(+3)_2\ Cu(+2)\ O(-2)_4$: undoped parent compound, d^9

$La(+3)_{2-x}\ Sr(+2)_x\ Cu(+2+x)\ O(-2)_4$: partially replacing La by Sr induces holes in Cu dx^2-y^2 orbital

dp model



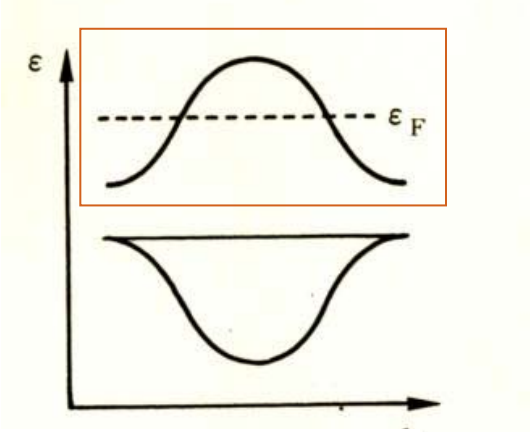
considers Cu3dx^2-y^2 and O2p orbitals that can hybridize with Cu3dx^2-y^2



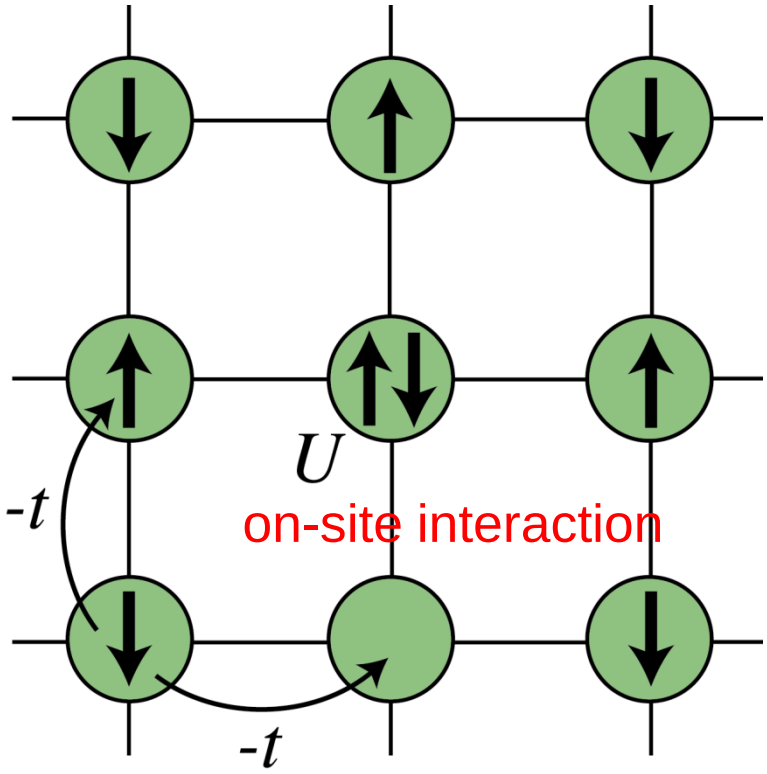
three sites per unit cell,
each site has one orbital
= three band model

Single band Hubbard model

consider only the band that intersects the Fermi level



single band model = single site per unit cell
one orbital per site

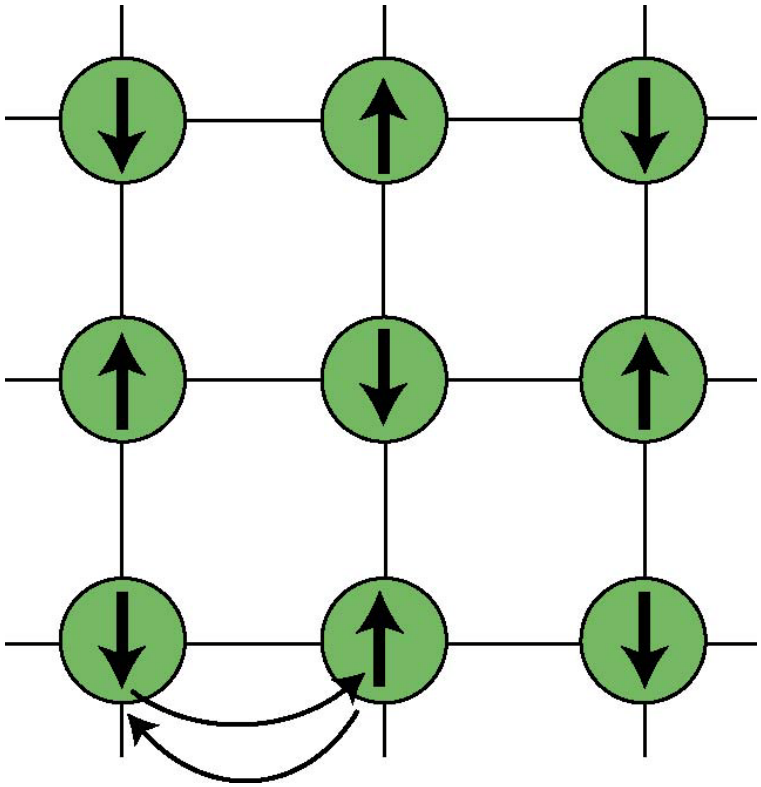


$t \sim 0.4$eV, $U \sim 8t$

undoped parent compound
= one electron / site =band filling (n) =1

Mott insulating state and antiferromagnetism

half-filled（undoped case）



Electrons are localized due to the on-site U : Mott insulator
In order to gain kinetic energy : antiferromagnetic spin ordering

Many body techniques

Quantum Monte Carlo method for finite size clusters
(up to O(100~1000) sites)

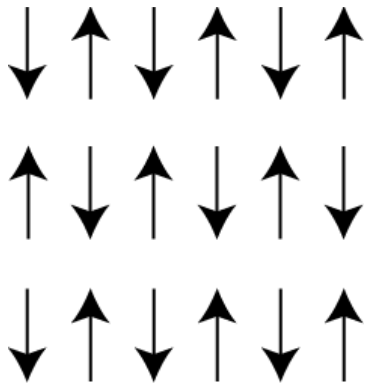
auxiliary field QMC

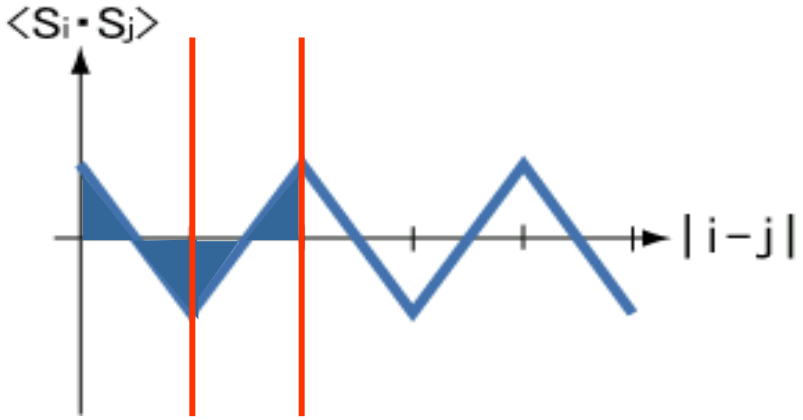
variational Monte Carlo

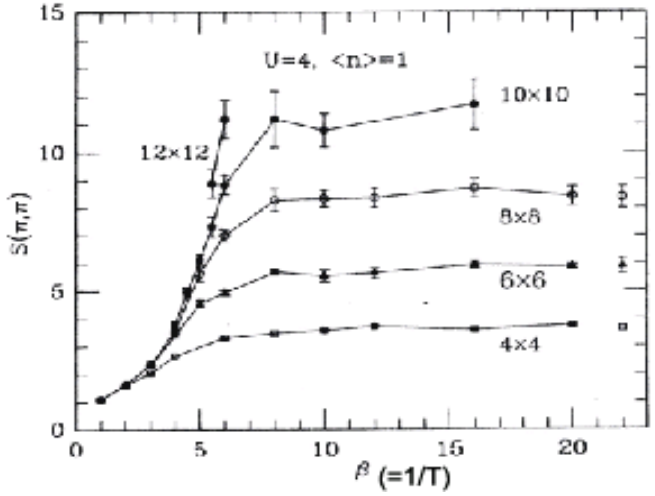
Diagrammatic approach

Combination

spin correlation function





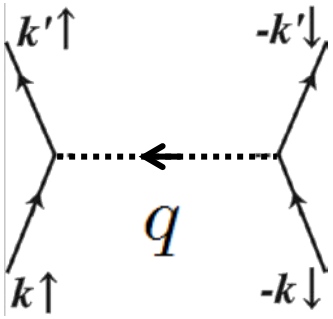


$$\frac{1}{N}\sum_{i,j}^{N}(-1)^{|i-j|}\left\langle S_i \cdot S_j \right\rangle$$

Spin correlation function calculated by AFQMC

White et al.Phys Rev.B40(1989) 506

Cooper pairing due to repulsive interaction ???

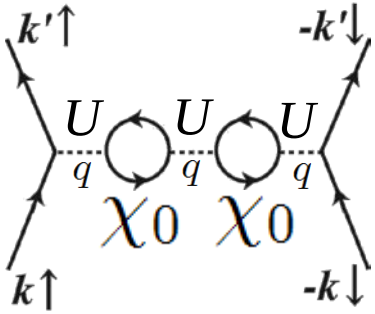


$$k' = k + q$$

gap equation

$$\Delta(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} \frac{\tanh[E(\boldsymbol{k}')/k_B T]}{2E(\boldsymbol{k}')} \underbrace{V\ (\boldsymbol{k}-\boldsymbol{k}')}_{\begin{array}{c}\| \\ U>0\end{array}} \Delta(\boldsymbol{k}')$$

this equation obviously does not have a finite gap solution



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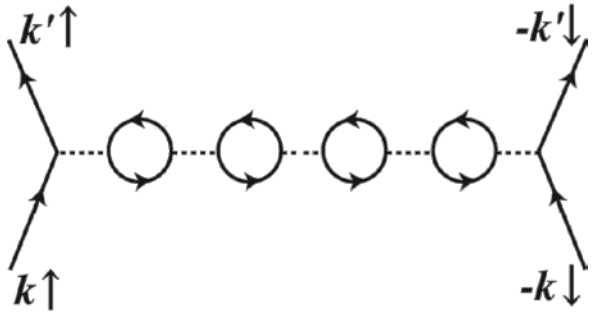
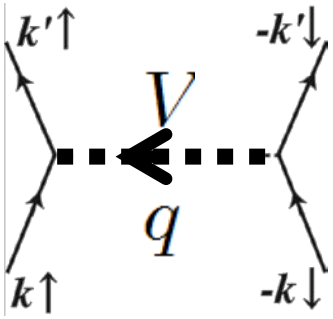


+ ⋯

collect contributions from certain types of diagrams

=



$$k' = k + q$$

effective pairing interaction

$$V(q) = \frac{U^3 \chi_0(q)^2}{1-(U\chi_0(q))^2} = \left\{ \frac{\chi_0(q)}{1-U\chi_0(q)} - \frac{\chi_0(q)}{1+U\chi_0(q)} \right\} U$$

bare susceptibility

$$\chi_0(q) = \sum_k \frac{f(\varepsilon(k+q)) - f(\varepsilon(k))}{\varepsilon(k) - \varepsilon(k+q)}$$

spin and charge susceptibilities
(in random phase approximation)

$$\chi_s(q) = \frac{\chi_0(q)}{1 - U\chi_0(q)} \qquad \chi_c(q) = \frac{\chi_0(q)}{1 + U\chi_0(q)}$$

Magnetic (spin) susceptibility

$$M = \chi H$$

$$M(\mathbf{q},\omega)\exp(i\mathbf{q}\cdot\mathbf{r} - i\omega t)$$

$$= \chi(\mathbf{q},\omega)H(\mathbf{q},\omega)\exp(i\mathbf{q}\cdot\mathbf{r} - i\omega t)$$

spin susceptibility without electron-electron interaction at ω=0

$$\chi_0(q) = \sum_k \frac{f(\varepsilon(k+q)) - f(\varepsilon(k))}{\varepsilon(k) - \varepsilon(k+q)}$$

RPA spin susceptibility with electron-electron interaction *U*

$$\chi_s(q) = \frac{\chi_0(q)}{1 - U\chi_0(q)}$$

expression is valid for $U\chi_0 < 1$

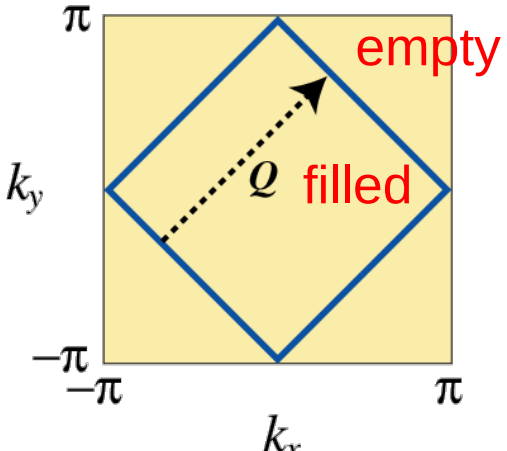
$$\chi_s(q) = \frac{\chi_0(q)}{1 - U\chi_0(q)} \rightarrow \infty \quad \text{as} \quad U\chi_0(q) \rightarrow 1$$

at a certain wavevector $q=Q$ where $\chi_0(q)$ is maximized

→magnetization for inifinitesimaly small magnetic field
→divergence of the susceptibility signals
spontaneous ordering of spins

for a fixed *U*, the divergence can occur by lowering the temperature ;
$\chi_0(q)$ can increase at certain wave vectors at low temperatures

Ideal square lattice, Fermi surface at half-filling : strongly nested



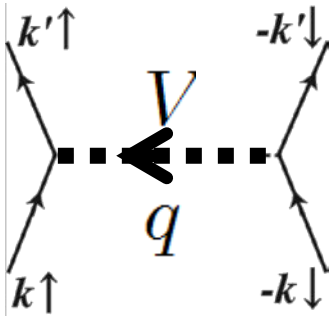
$$\frac{f(\varepsilon(k+q)) - f(\varepsilon(k))}{\varepsilon(k) - \varepsilon(k+q)}$$

is large at the nesting vector $q=Q$ when
f is close to a step function

sponteneous spin ordering (antiferromagnetism)
with a wave vector Q can take place at low temperature
when the Fermi surface is strongly nested

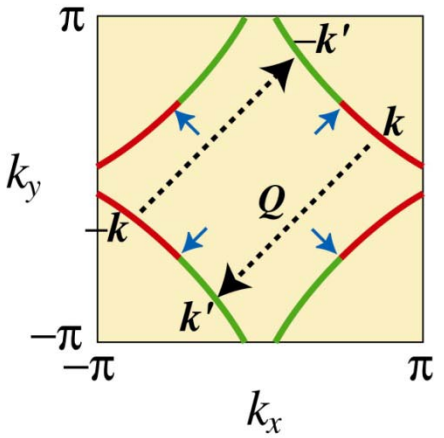
even when the Fermi surface nesting is degraded (by carrier doping for instance), large $\chi_s(Q)$ (spin fluctuations) remains

large $V(Q) > 0$



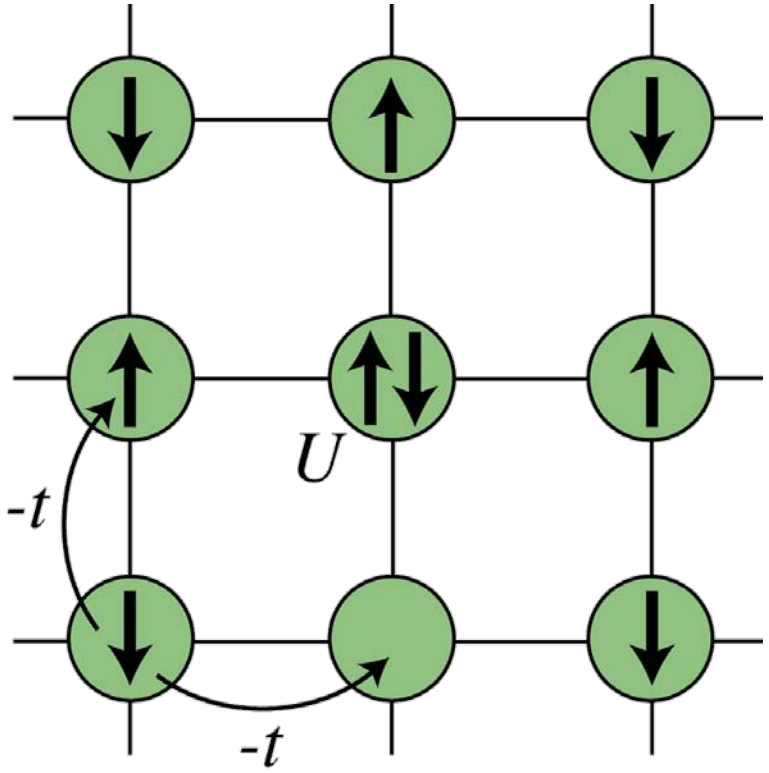
condition for SC : $V(\boldsymbol{k}-\boldsymbol{k}')\Delta(\boldsymbol{k})\Delta(\boldsymbol{k}') < 0$

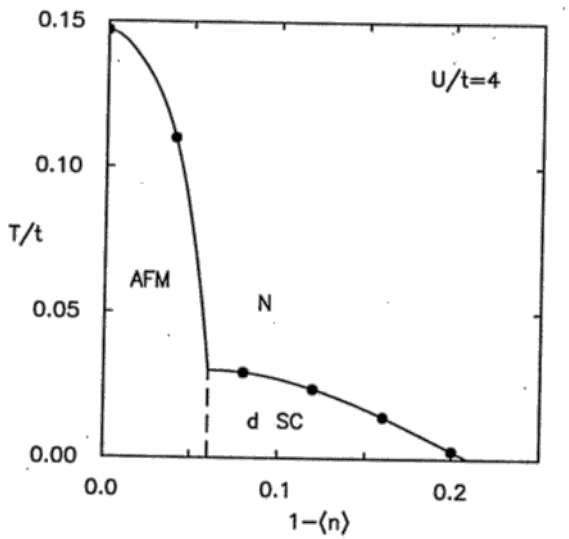
pairing int. mediated by spin fluctuation at $\boldsymbol{q}=\boldsymbol{Q}$
→SC gap $\Delta(\boldsymbol{k}) = -\Delta(\boldsymbol{k}+\boldsymbol{Q})$
→d-wave pairing



d-wave SC on square lattice

calculate the pairing interaction and
solve the gap equation for O(1000)～O(10000) lattice sites



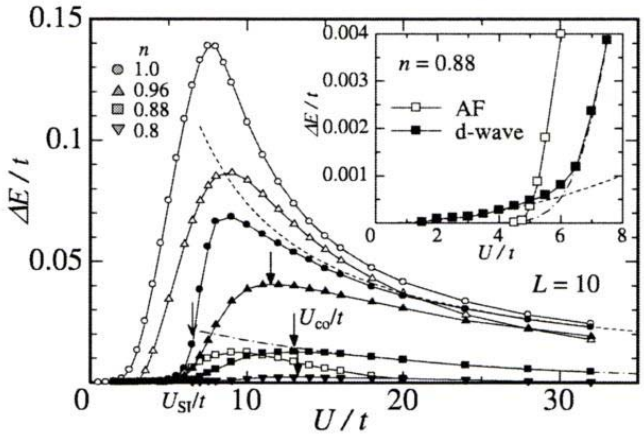


Bickers et al, PRB **43** (1991) 8044

d_{x2-y2}-wave SC T_c~O(0.01t)

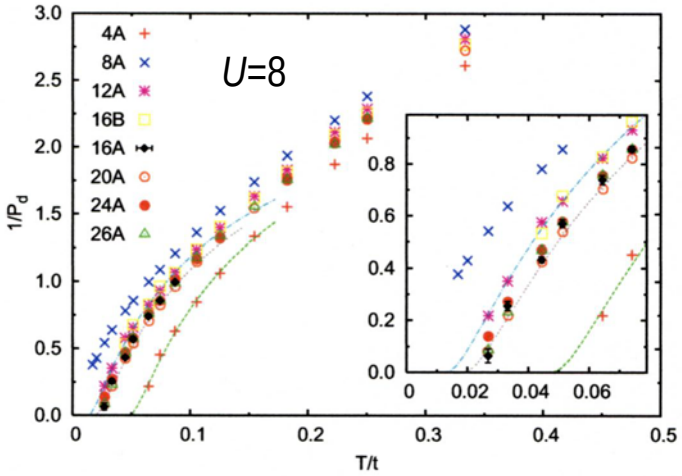
Other approaches for d-wave superconductivity in the Hubbard model

energy gain due to d-wave superconductivity
Variational Monte Carlo (VMC)



Yokoyama, Tanaka, Ogata, Tsuchiura JPSJ **73** (2004) 1119

inversed SC susceptibility by
Dynamical Cluster Approximatoin (DCA)



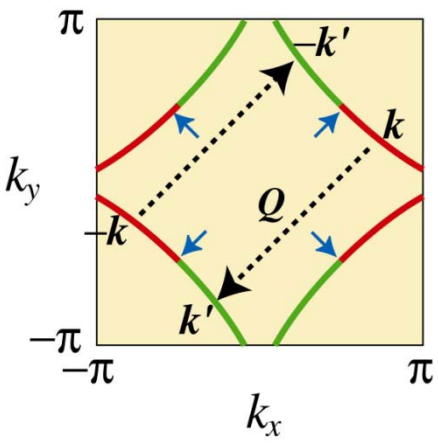
T.A. Maier et al, PRL 95 (2005) 237001

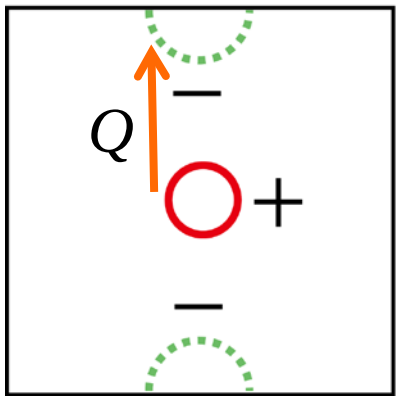
d_{x2-y2}-wave SC $T_c \sim O(0.01t)$

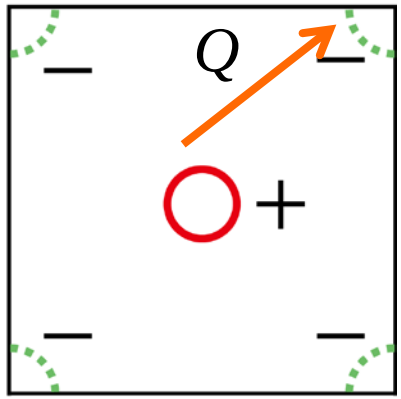
T_c =O(10)K～100K

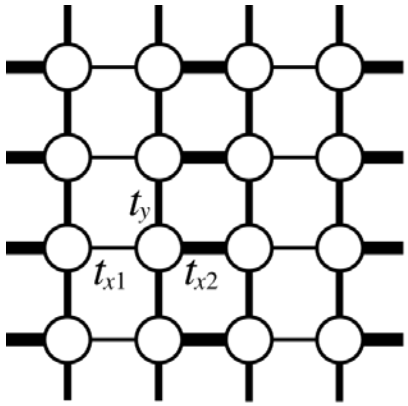
high Tc, but still “low Tc” compared to the energy scale of t (kinetic energy of electrons)

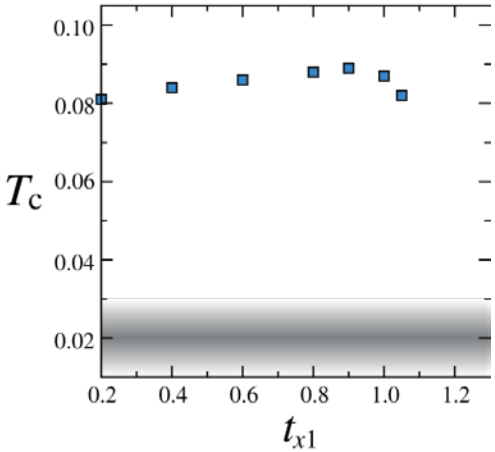
HTC spin fluctuation mediated pairing from disconnected Fermi surfaces : single orbital case











U = 8, ty = 1, tx2 = 1.2 in units of tx1

KK and R. Arita, PRB 2001,2002
Bulut et al PRB 1992
Maier & Scalapino arXiv:11070401

Discovery of SC in LaFeAsO

Published on Web 02/23/2008

Iron-Based Layered Superconductor La[$O_{1-x}F_x$]FeAs ($x = 0.05-0.12$) with $T_c = 26$ K

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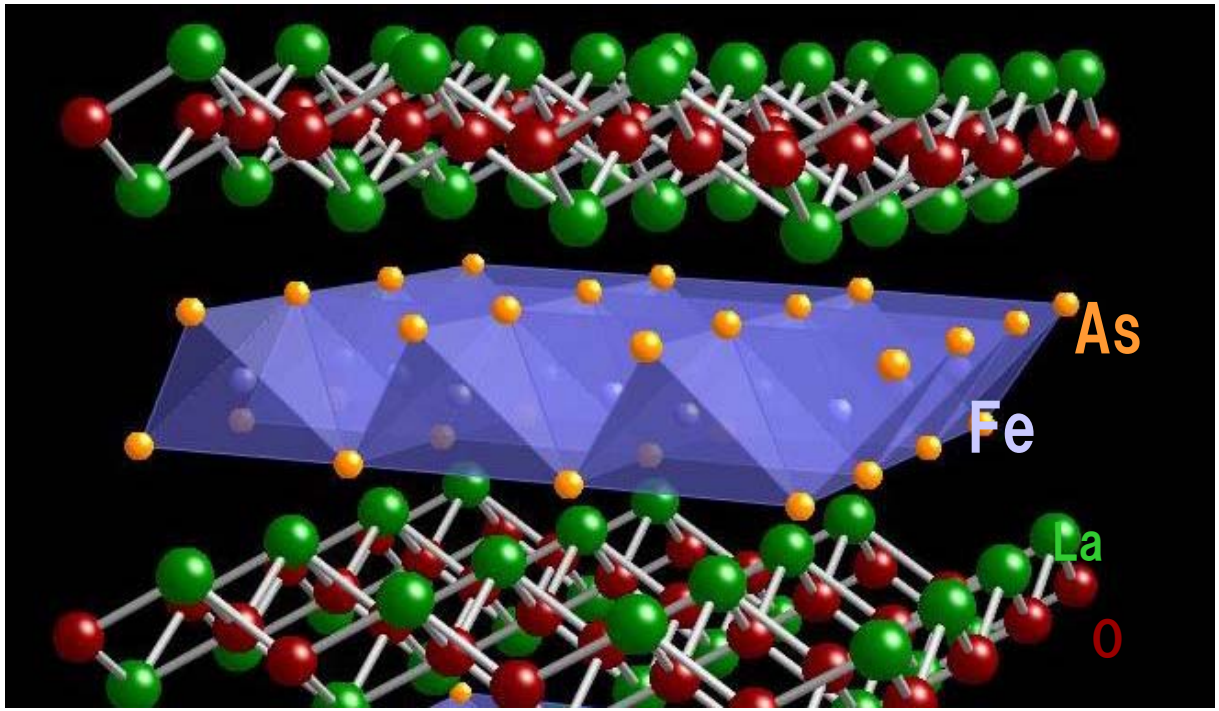
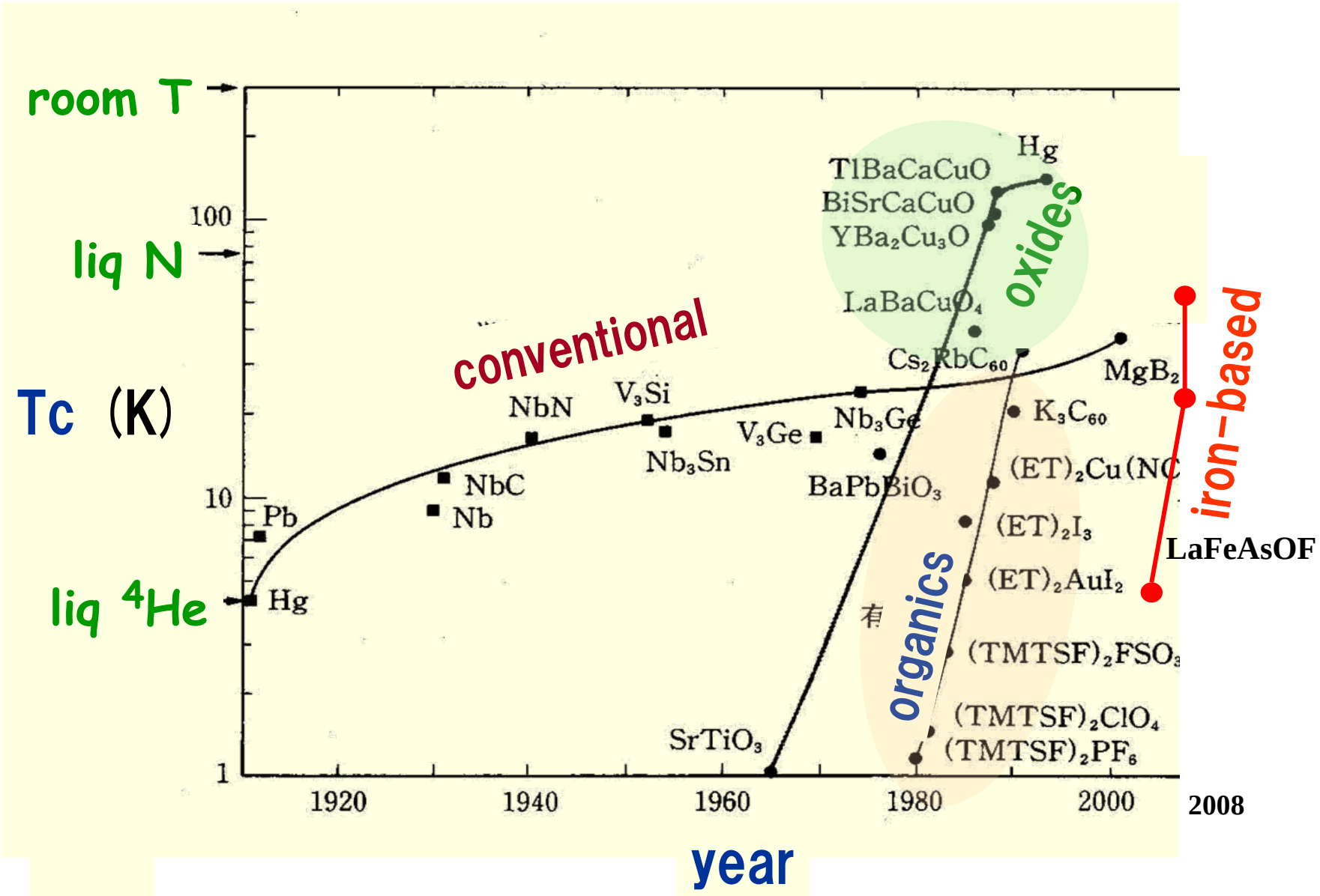
ERATO-SORST, JST, Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-1, and Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

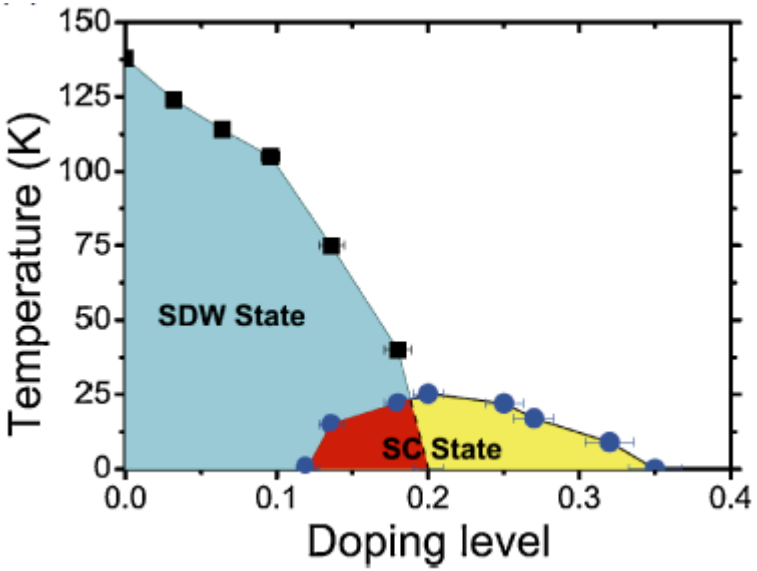
Received January 9, 2008; E-mail: hosono@msl.titech.ac.jp



High Tc up to 55 K by La->Sm,Nd

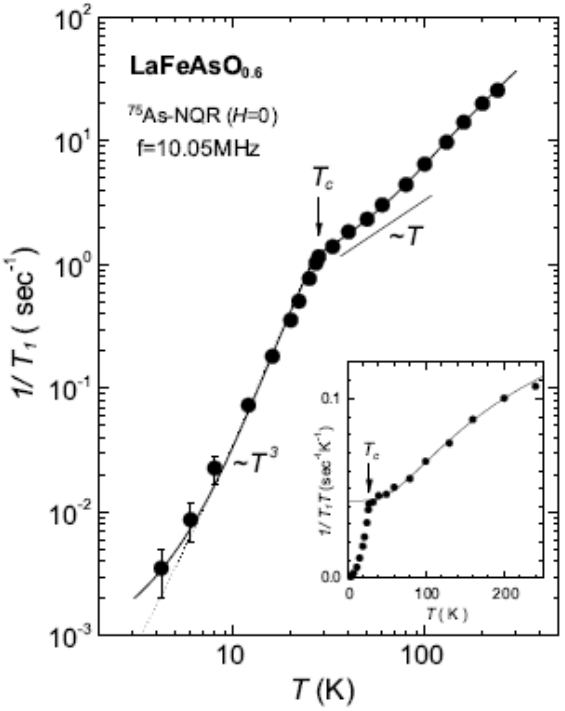


Possible unconventional pairing



X.F. Wang et al

magnetism near superconductivity



H. Mukuda et al

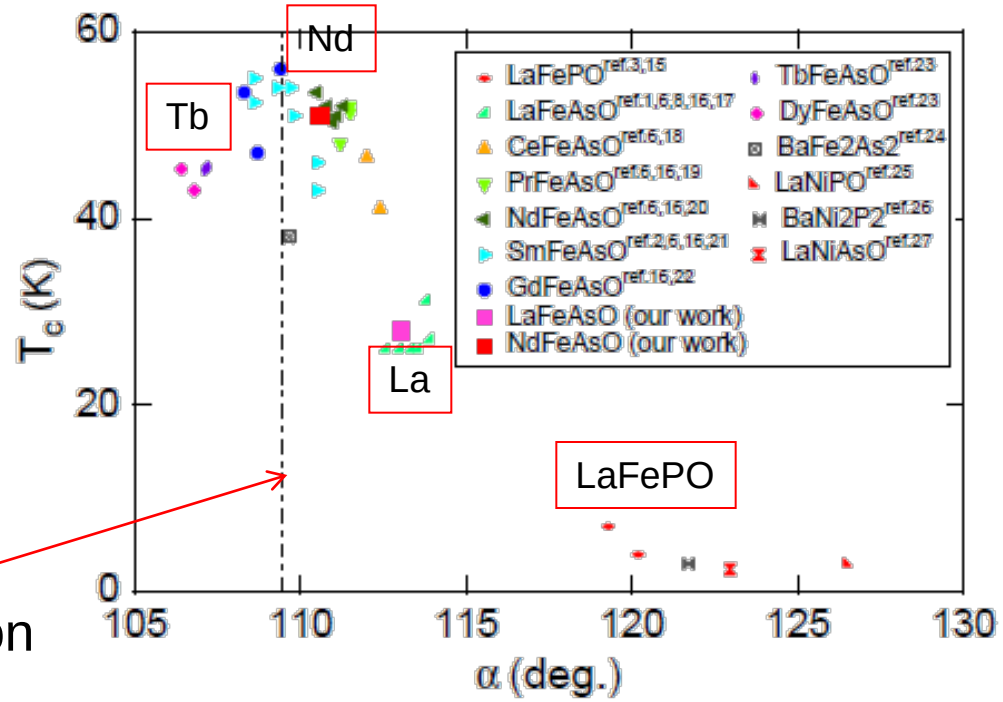
no coherence peak, NQR

First principles calculation :

electron phonon coupling too weak for Tc=50K

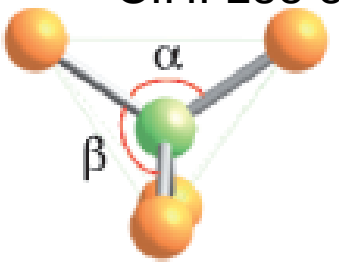
Boeri et al

Material dependence of Tc in iron pnictides



regular tetrahedron

C.H. Lee et al, JPSJ **77** (2008) 083704

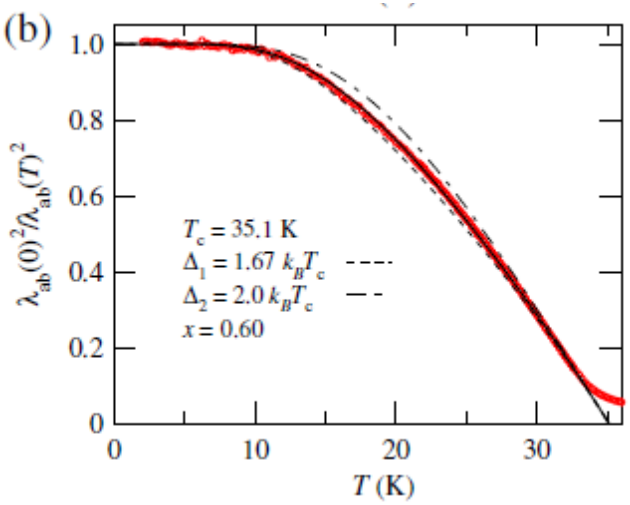


FeAs$_4$-tetrahedron

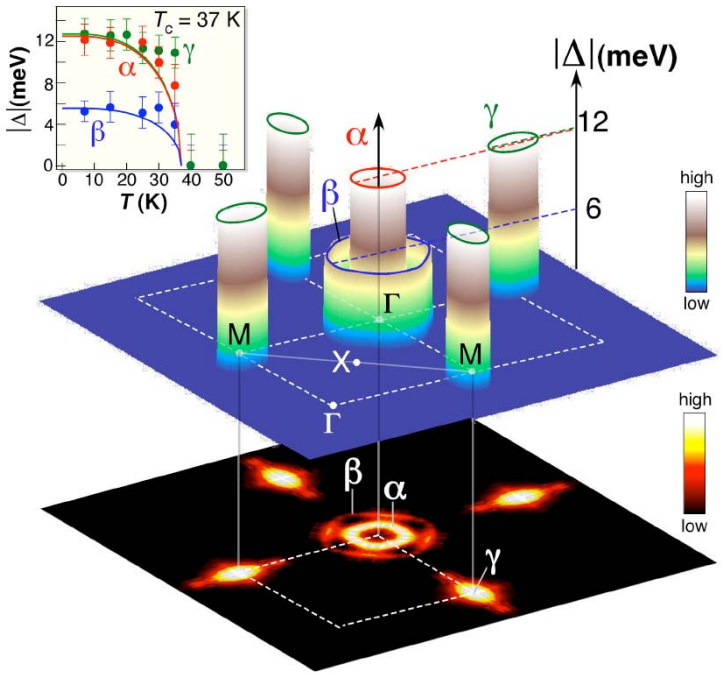
also by J. Zhao, Nat. Mat. 7, 953 (2008)

Material dependence of SC gap

a number of experiments suggest fully open gap (with multiple gaps or anisotropy) for the arsenides,



Hashimoto et al,
penetration depth PrFeAsO

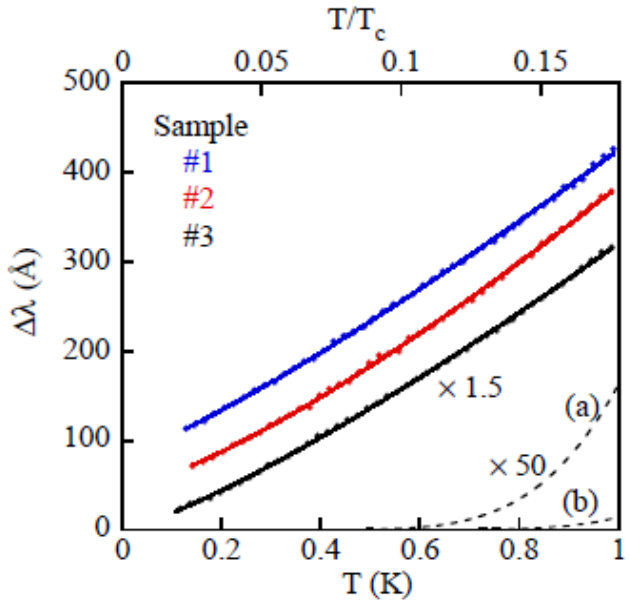


Ding et al, Ba122, ARPES

Material dependence of SC gap

for LaFePO (Tc~5K), experiments
show presence of line nodes in the SC gap

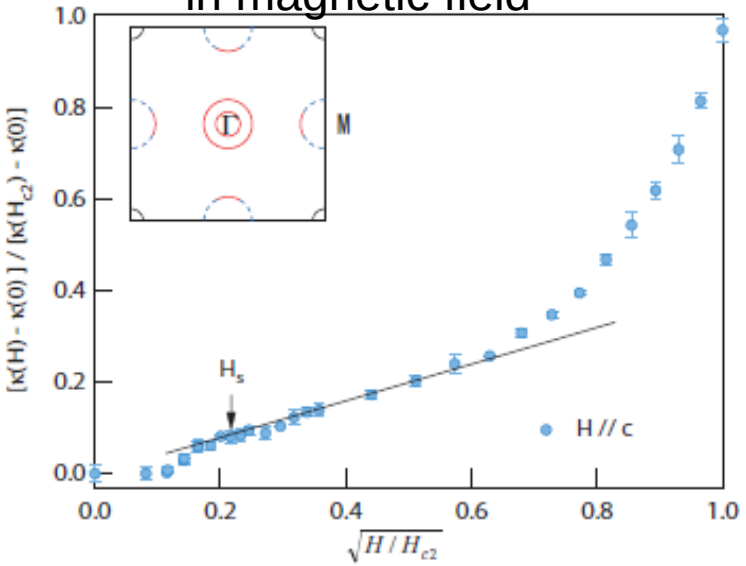
penetration depth



Fletcher et al, PRL **102**, 147001 (2009)

also Hicks et al., PRL 2009

thermal conductivity
in magnetic field



M. Yamashita et al., PRB 2010

Material Specific Hamiltonian for studying unconventional SC

lattice structure, elements

first principles band calculation (pwscf, Wien2K)

maximally localized Wannier orbitals (wannier90)

material specific tight binding model

Fermi surface multiplicity, shape, orbital weights

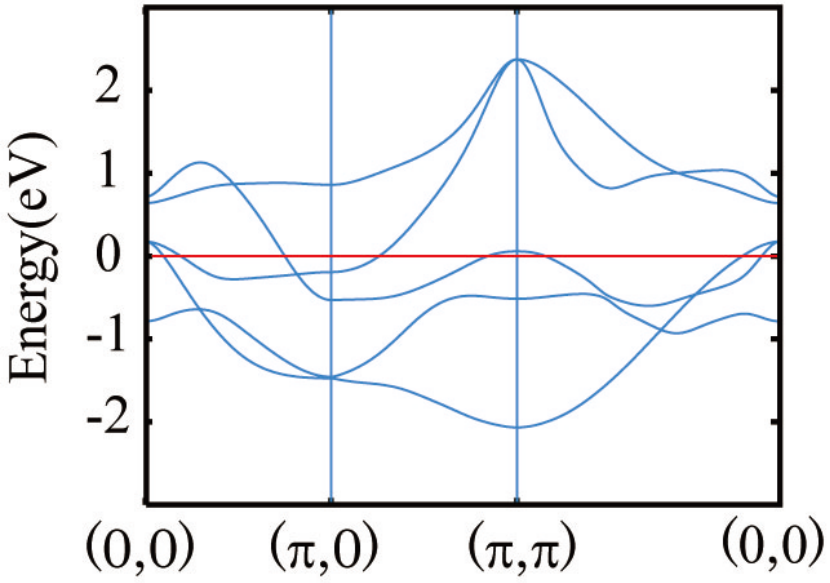
\+

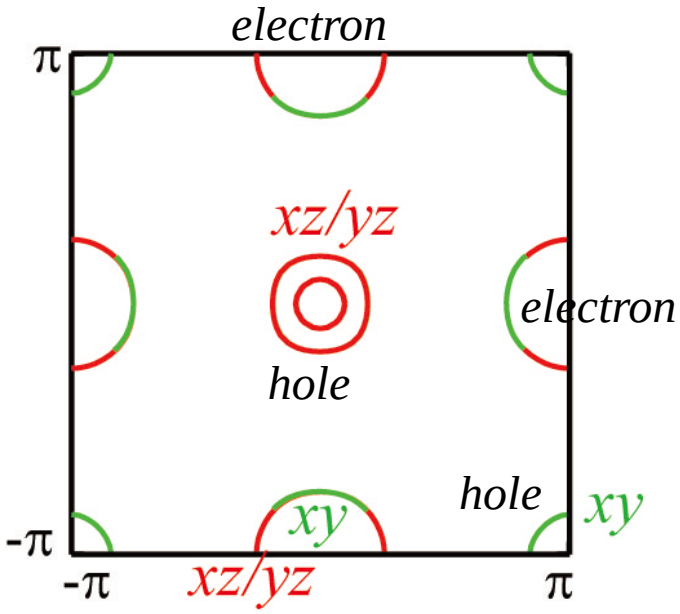
Superconductivity

electron-electron interaction

Five orbital model

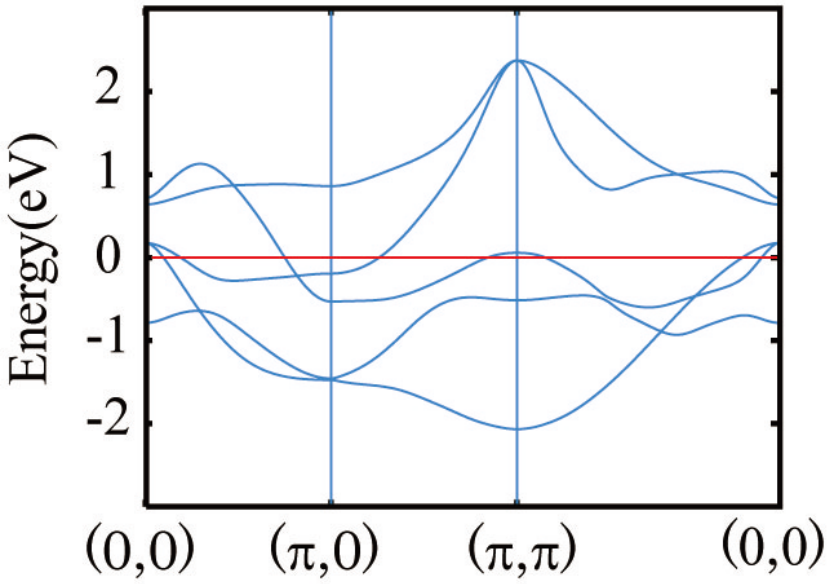
all five iron 3d orbitals are necessary to correctly reproduce the band structure and the Fermi surface

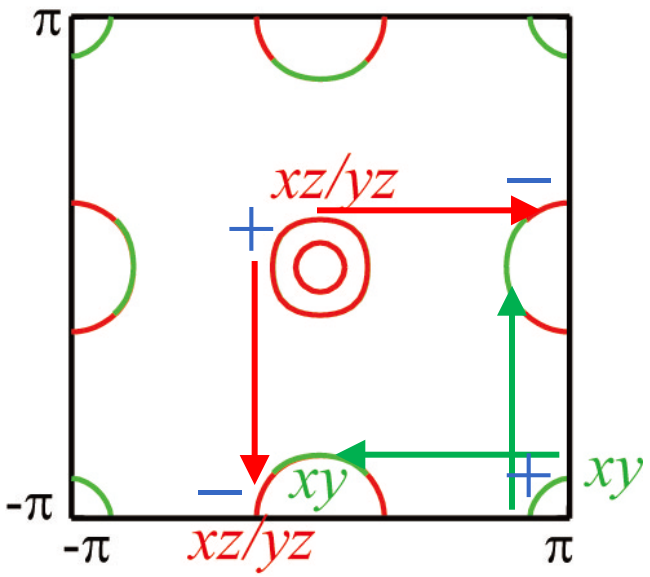




Fermi surface nesting and "s±" SC

pairing int. mediated by spin fluctuation at $\boldsymbol{q}=\boldsymbol{Q}\rightarrow$ SC gap $\Delta(\boldsymbol{k})= -\Delta(\boldsymbol{k}+\boldsymbol{Q})$



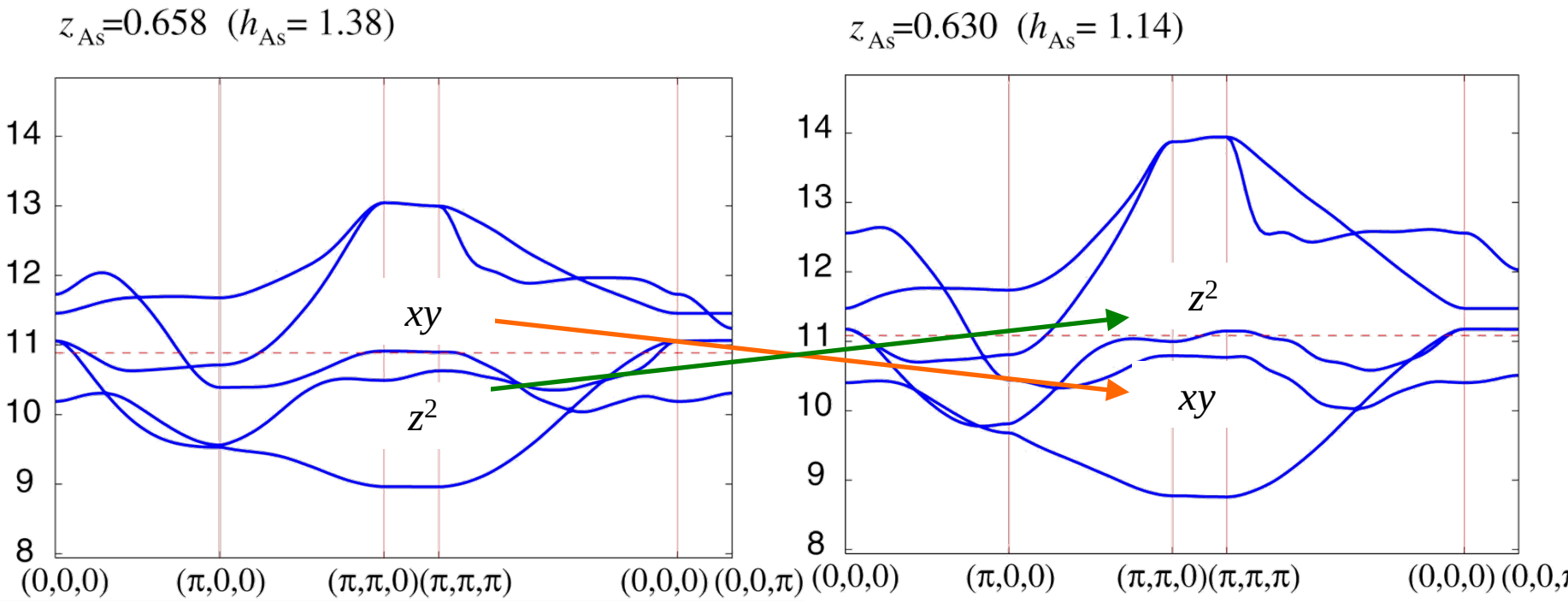


two types of $(\pi,0)$ spin fluctuations originating from different orbitals cooperating

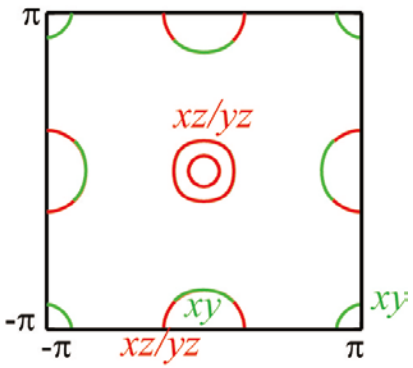
fully gaped "s±" Mazin et al PRL 2008

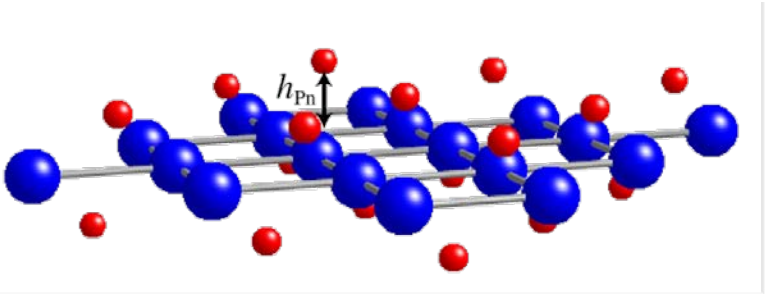
high

low



KK et al., PRB **79** (2009) 224511





Effective Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

$$\mathcal{H}_0 = \sum_{ij}\sum_{\mu\nu}\sum_{\sigma} t_{ij}^{\mu\nu} c_{i\mu\sigma}^{\dagger} c_{j\nu\sigma} + \sum_{i\mu\sigma} \epsilon_{\mu} n_{i\mu\sigma}$$

i, j: site、μ, ν: orbitals

$$\mathcal{H}_1 = \sum_{i} \left[U \sum_{\mu} n_{i\mu\uparrow} n_{i\mu\downarrow} + U' \sum_{\mu>\nu} n_{i\mu} n_{i\nu} + J \sum_{\mu\neq\nu} \boldsymbol{S}_{i\mu} \cdot \boldsymbol{S}_{i\nu} + J' \sum_{\mu\neq\nu} c_{i\mu\uparrow}^{\dagger} c_{i\mu\downarrow}^{\dagger} c_{i\nu\downarrow} c_{i\nu\uparrow} \right]$$

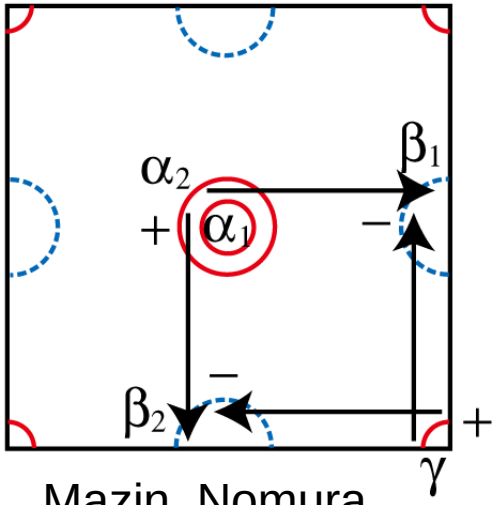
apply multi-orbital random phase approximation :
typically, ～50×50×10 sites × 5 orbitals ～ 10^4 ～ 10^5 orbitals

pnictogen height dependent sc gap

high

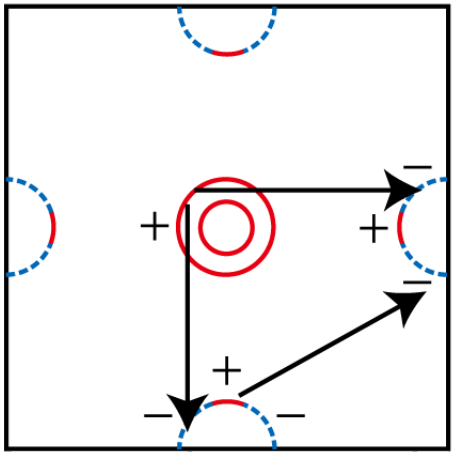
low

fully gapped $s\pm$wave



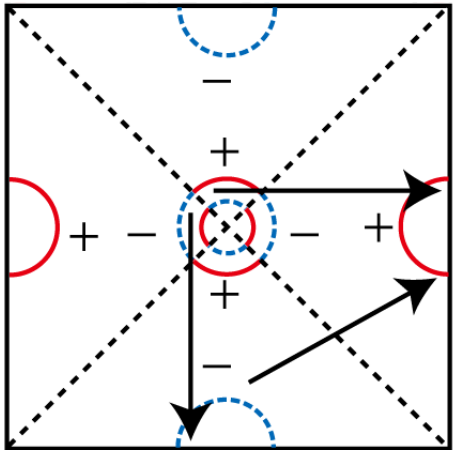
Mazin, Nomura, Ikeda, Wang, KK, Chubukov, Ji, Daghofer….

nodal $s\pm$wave



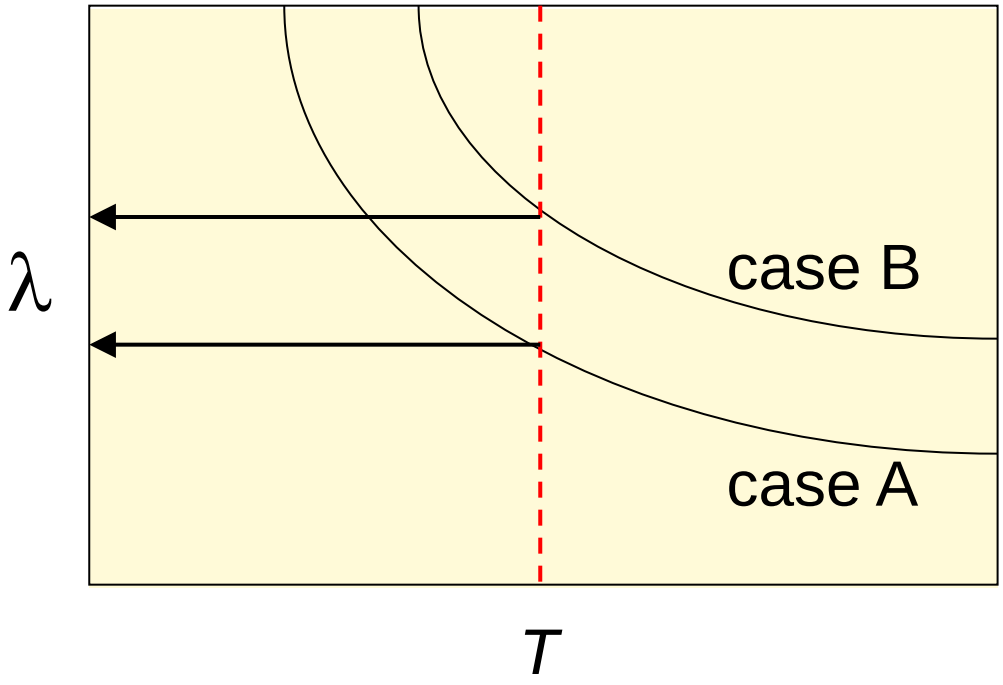
Graser et al.
Mishra et al.
KK et al.
Wang et al.
Thomale et al

d-wave



KK et al.,
Graser et al,
Yanagi
Ikeda&Arita…

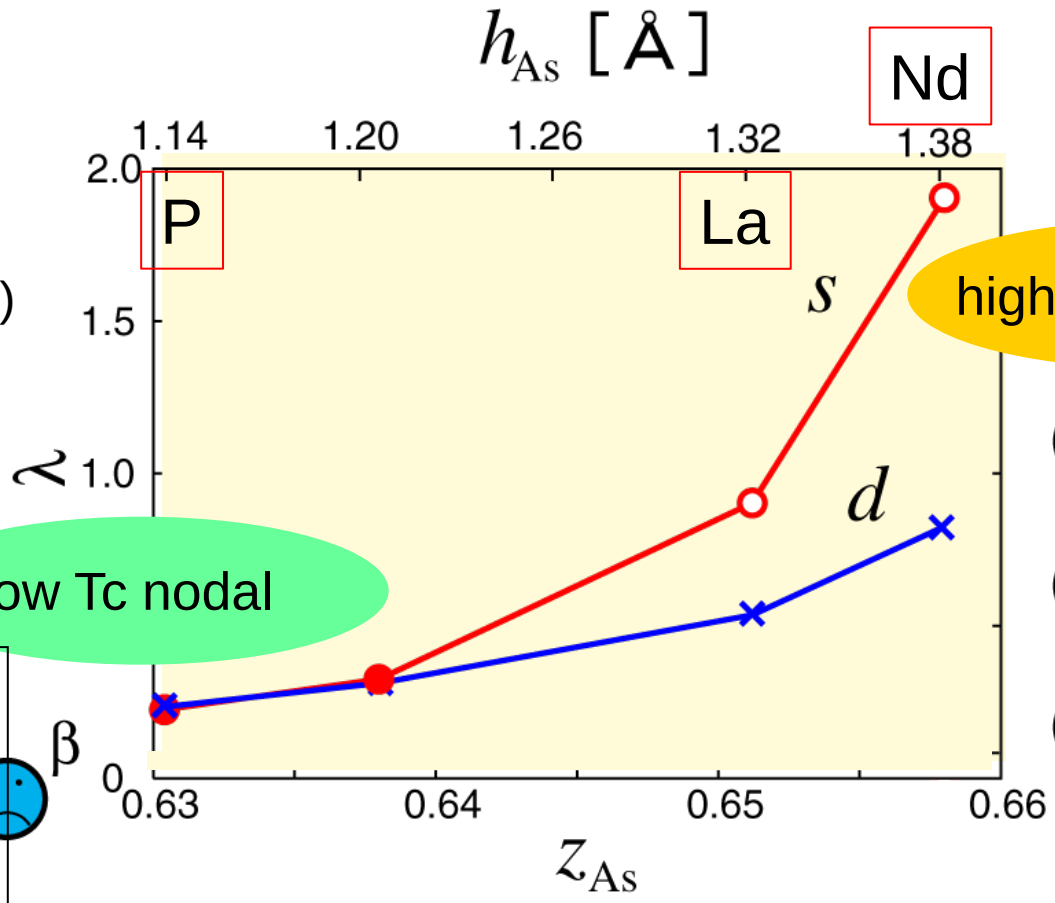
Linearized gap equation



λ at a fixed *T* can used as a qualitative measure for Tc

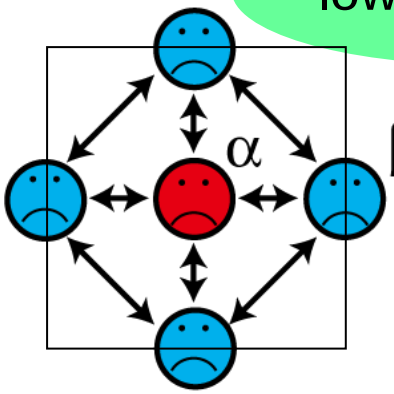
“Height” as a switch between high Tc nodeless and low Tc nodal pairings

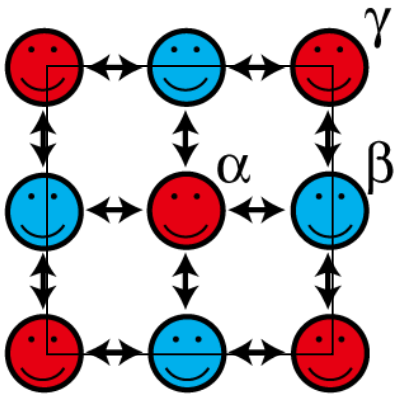
U=1.2, U’=0.9,
J=J’=0.15
n=6.1 (10% dope)
T=0.02 (eV)



high Tc nodeless

low Tc nodal

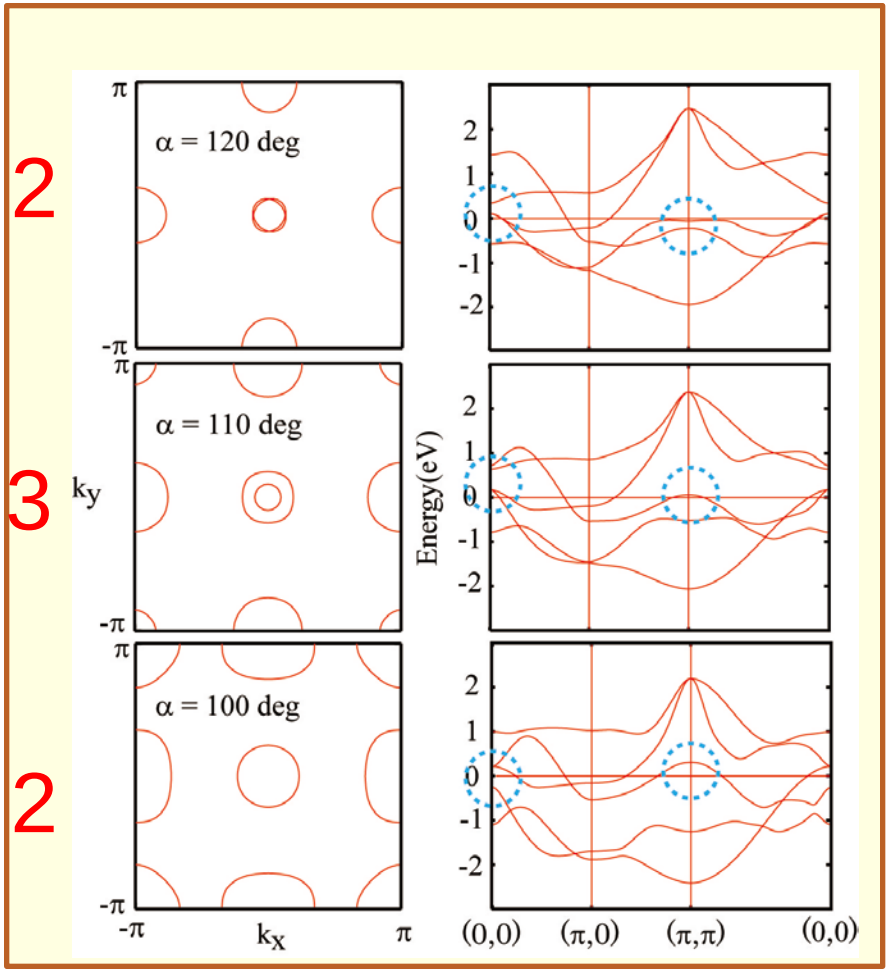




KK et al., PRB **79** (2009) 224511

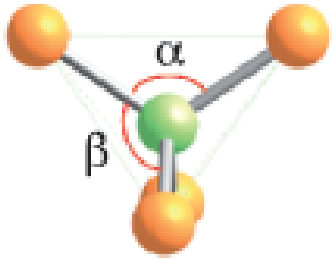
Bond angle dependence of Fermi surface multiplicity

FS for 10% doping



H. Usui and KK, PRB 84 (2010) 024505

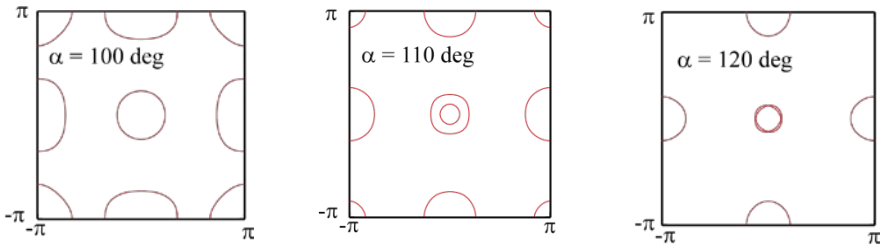
Fe-As bond length= fixed



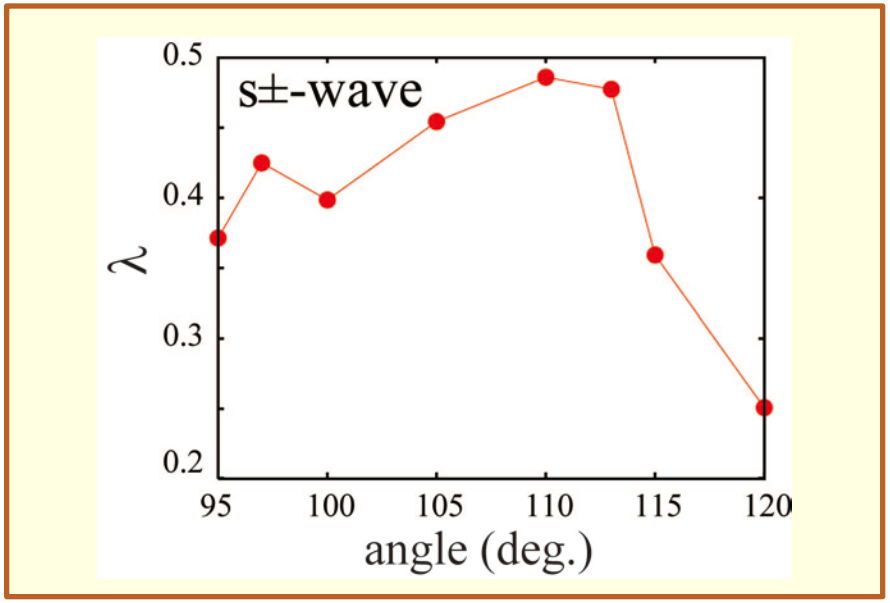
$FeAs_4$-tetrahedron

This kind of Fermi surface variation first found in T. Miyake et al, JPSJ **79** (2010) 123713

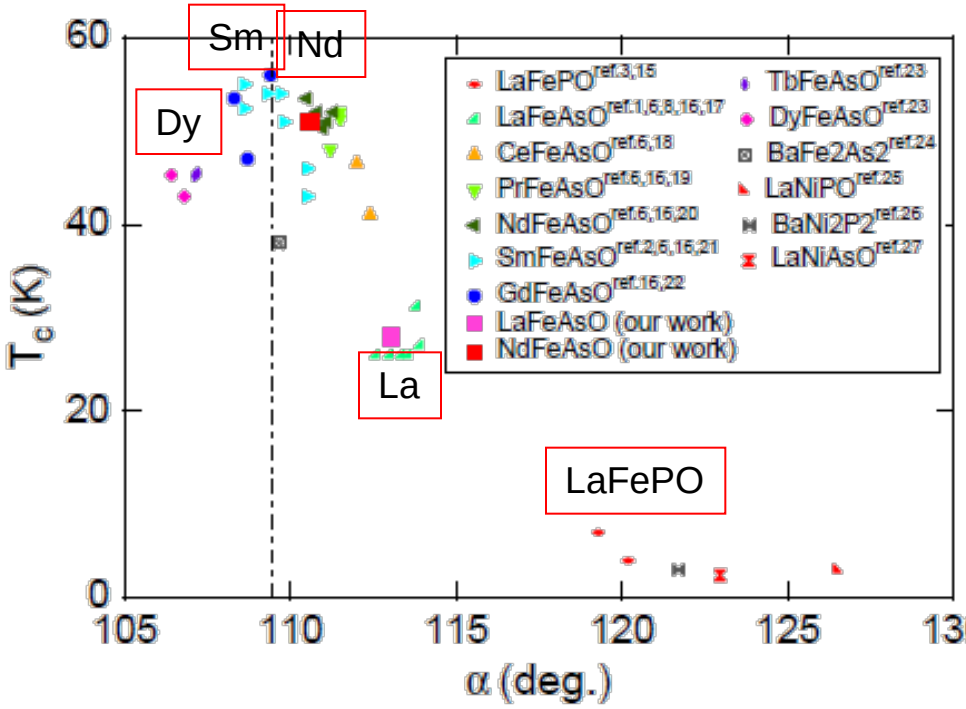
Bond angle dependence of SC



T=0.005eV



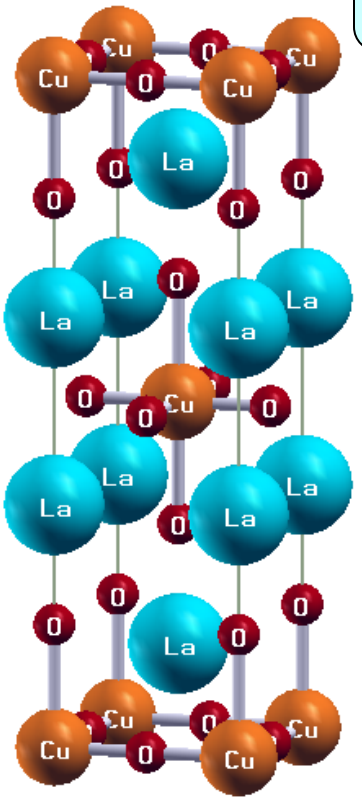
H. Usui and KK, PRB 84 (2010) 024505



C.H. Lee et al, JPSJ **77** (2008) 083704

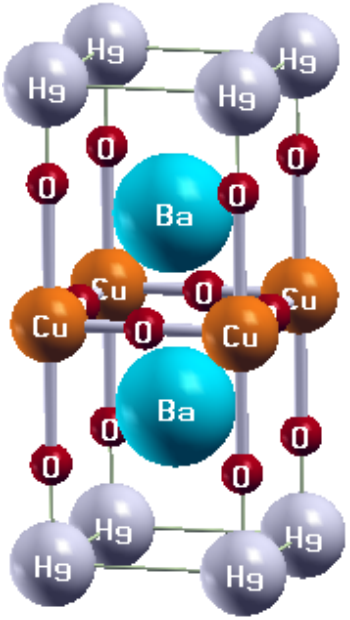
Material dependence of Tc in cuprates

Single layer system



La

Hg

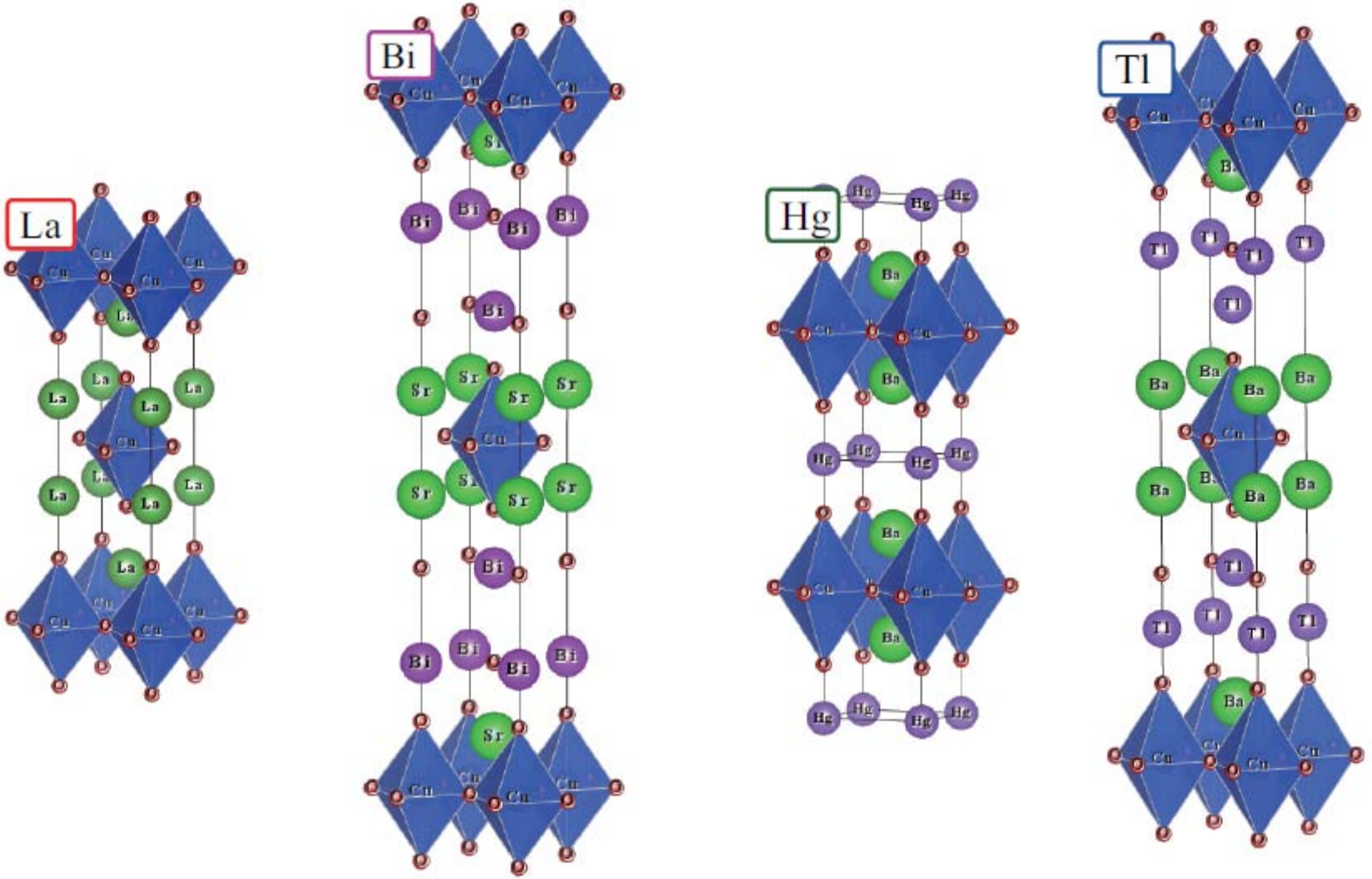


La_2CuO_4 (T_c～40K)

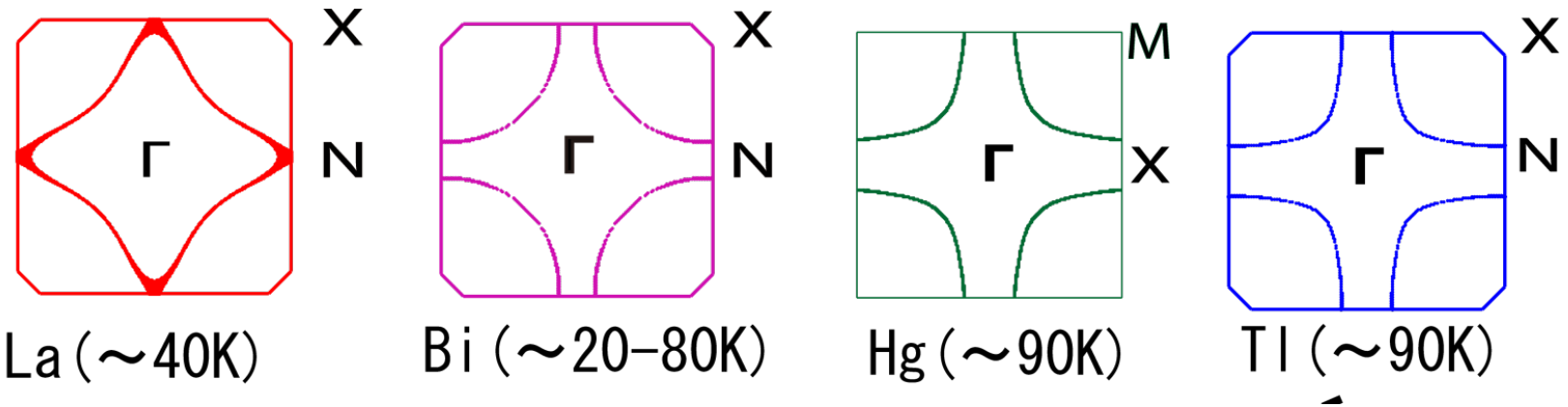
low

high

$HgBa_2CuO_4$ (T_c～90K)


La
Bi
Hg
Tl

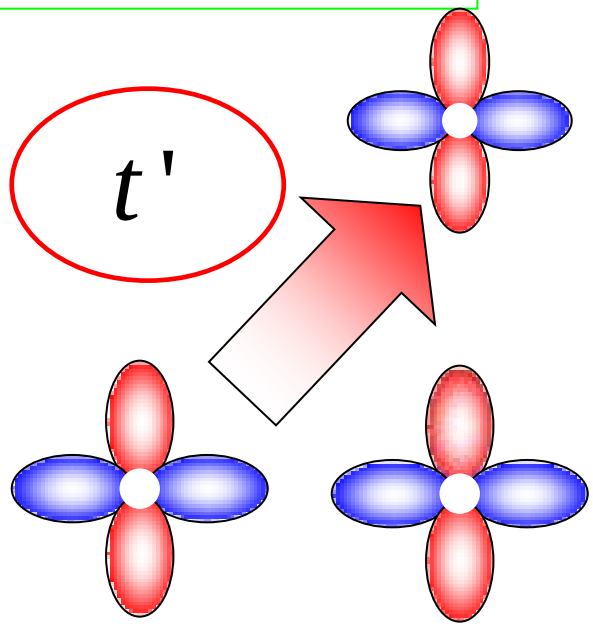
Fermi surface shape and Tc

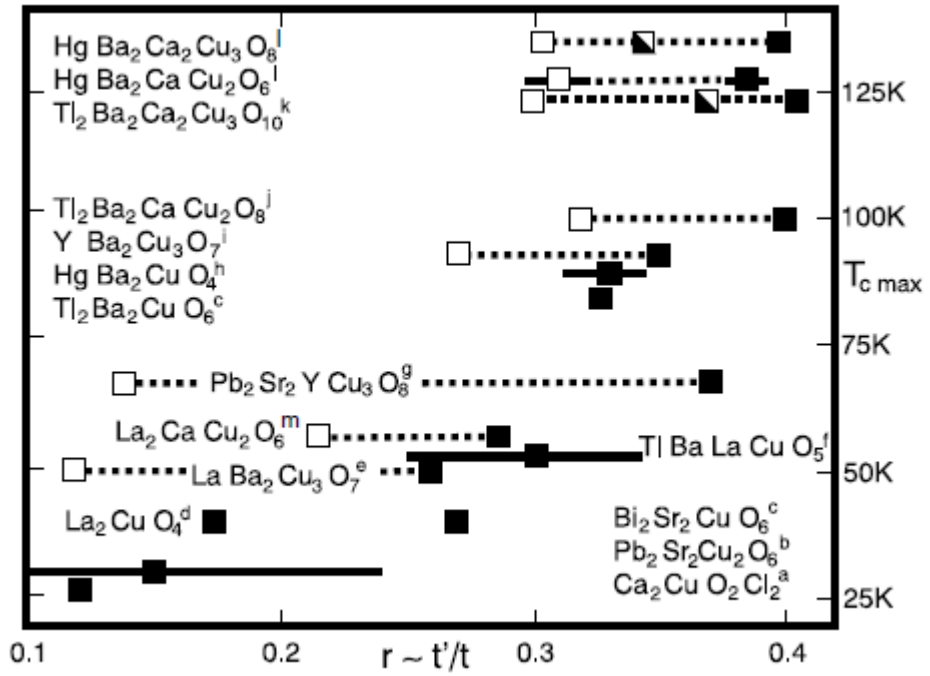


stronger Fermi surface roundness ("larger *t'* ") → higher Tc

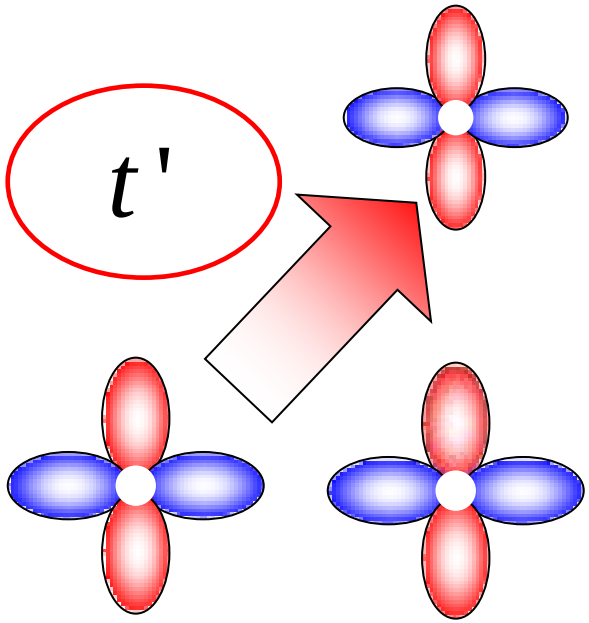
E. Pavarini, *et al,* PRL **87**.047003(2001)

K. Tanaka, *et al,* PRB **70**.092503(2004)





E. Pavarini, *et al,* PRL **87**.047003(2001)

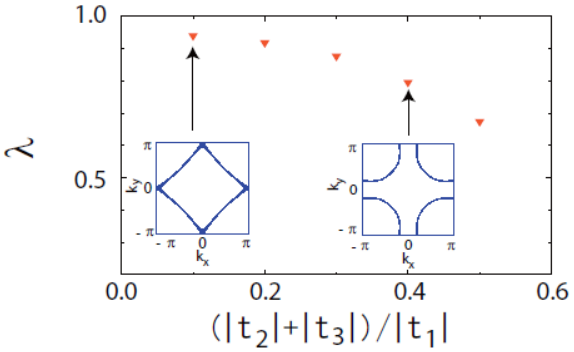


Fermi surface shape and Tc : theory

FLEX, single band Hubbard

microscopic theories for Hubbard type models

stronger Fermi surface roundness →lower Tc



SCR theory : explains material dependence

T.Moriya & K. Ueda 1994

t-J model or large U Hubbard model;

larger t' → favorable for superconductivity

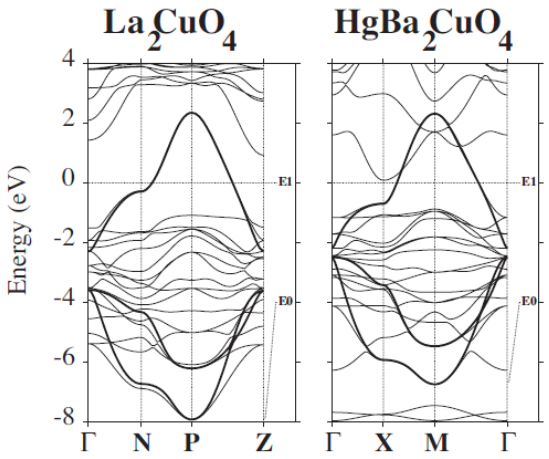
C.T. Shih et al 2004, P. Prelovsek&A. Ramsak 2005 , H.Yokoyama and M.Ogata

DCA for d-p model

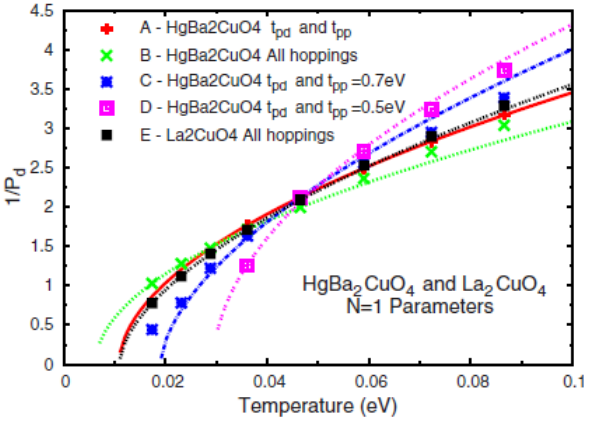
Kent et al, 2008

Tc La > Hg

(for all hoppings)



inversed SC susceptibility

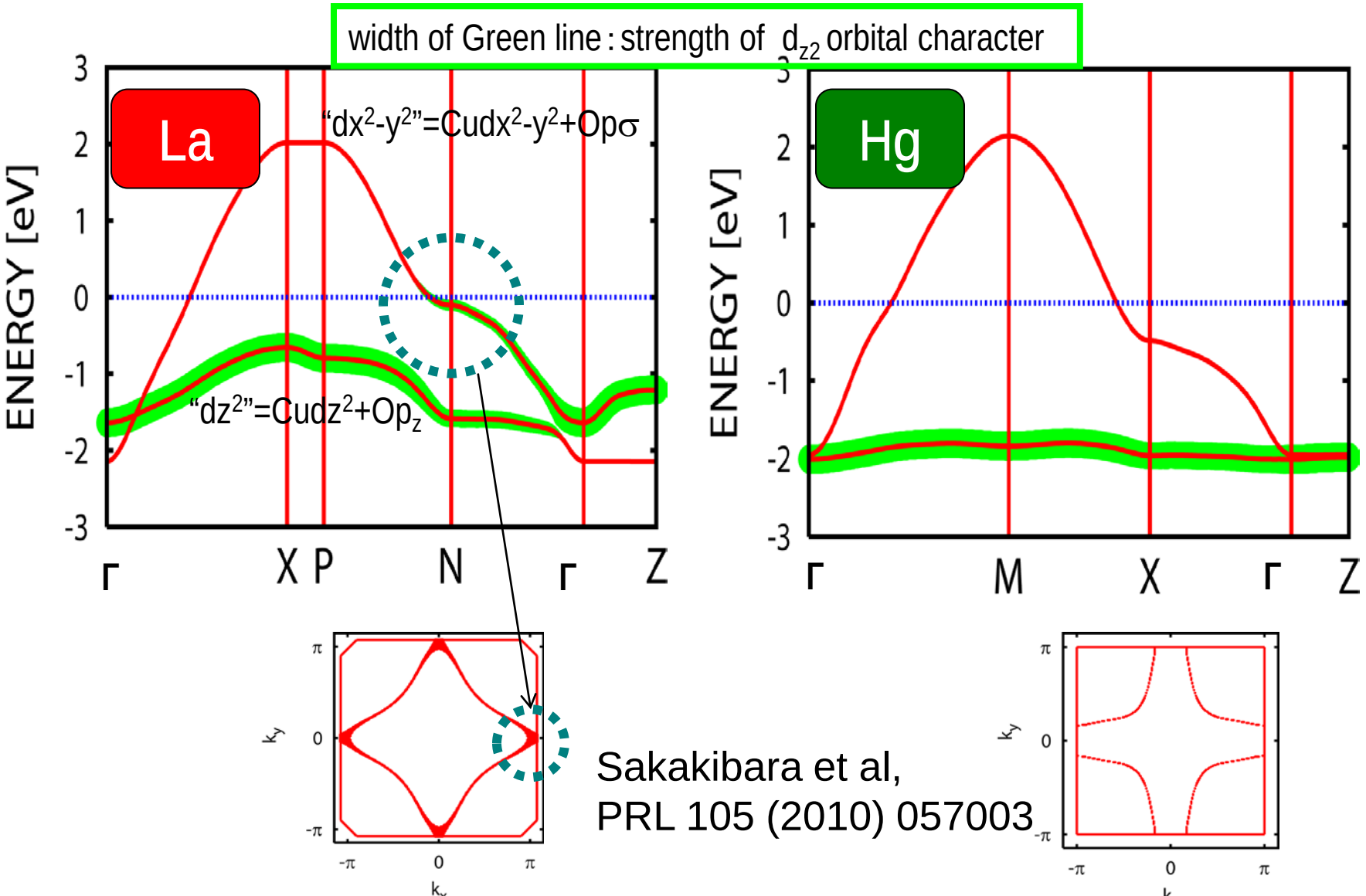


dx^2-y^2 +dz^2 two orbital model

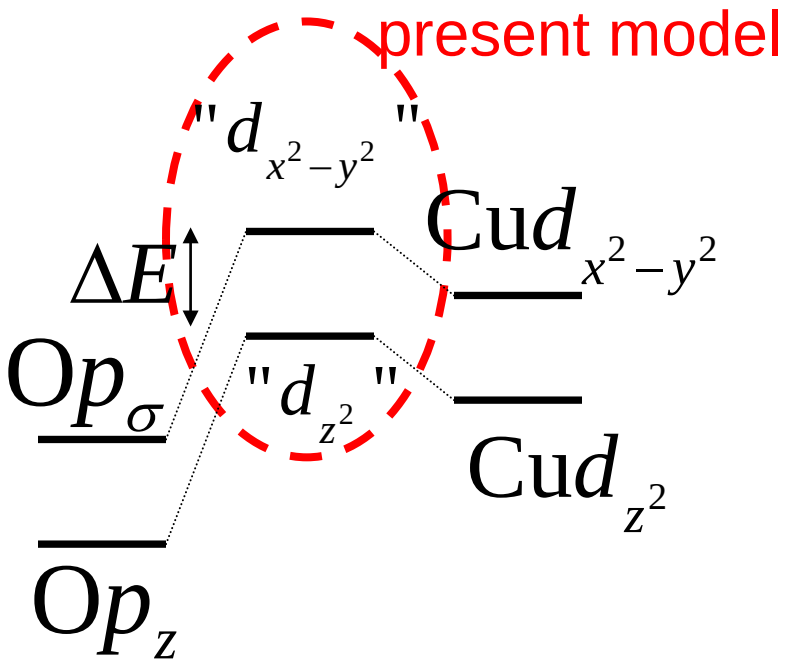
importance of the dz^2 orbital:

H. Kamimura et al 1990, C.DiCastro 1991

O.K.Andersen et al J. Phys. Chem. Solids 1995, E.Pavarini et al PRL 2001

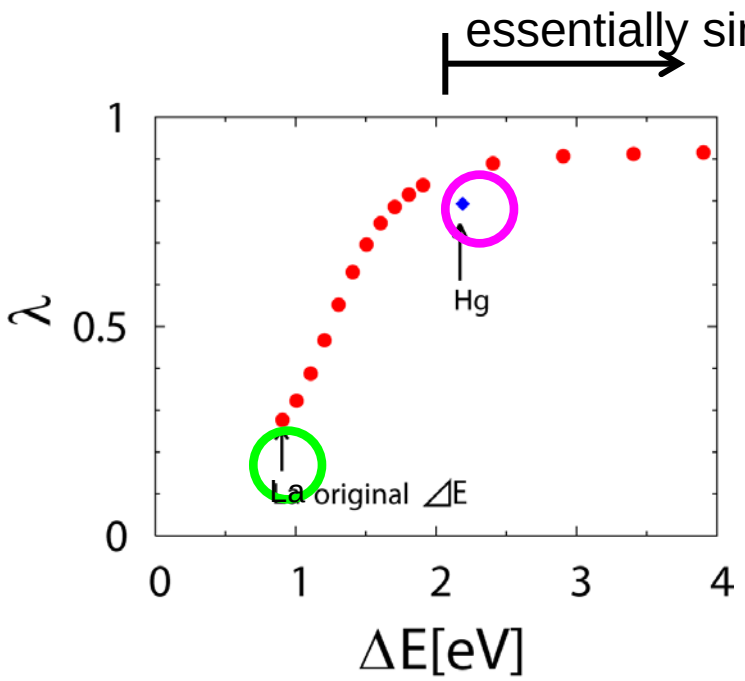


Energy level diagram



$$\Delta E = E^{on-site}_{x^2-y^2} - E^{on-site}_{z^2}$$ ⇒ measures the contribution of the d_{z2} orbital to the Fermi surface

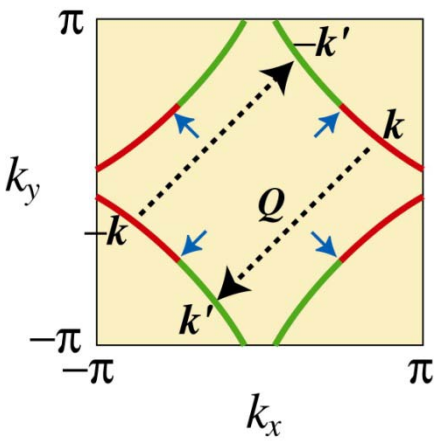
Correlation between Tc and ΔE

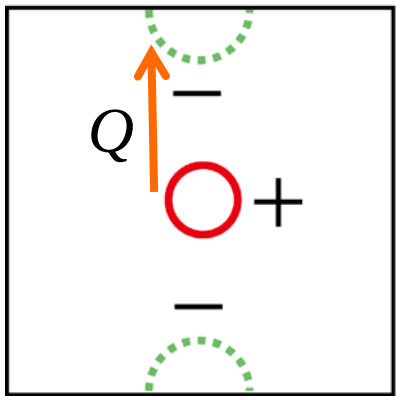


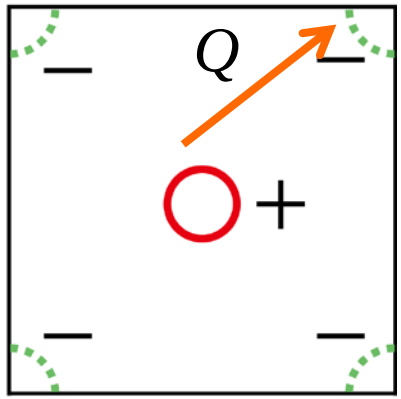
Sakakibara et al, 2010

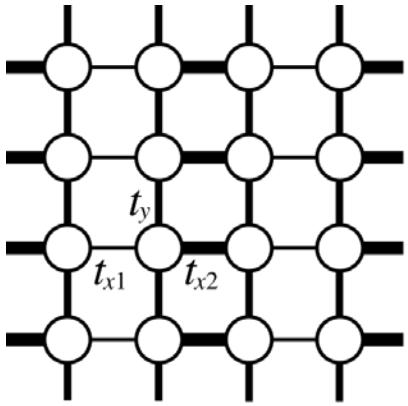
vary ΔE directly “by hand”
in the two orbital model of La214

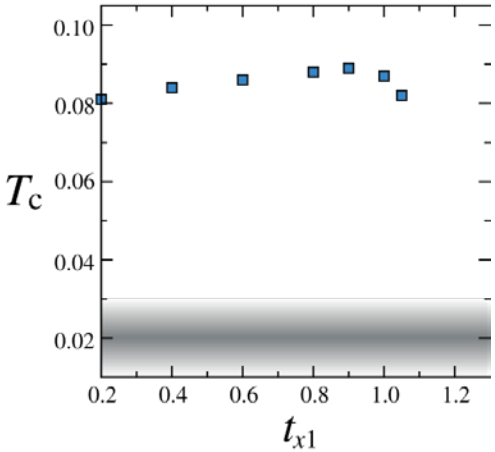
HTC spin fluctuation mediated pairing from disconnected Fermi surfaces : single orbital case







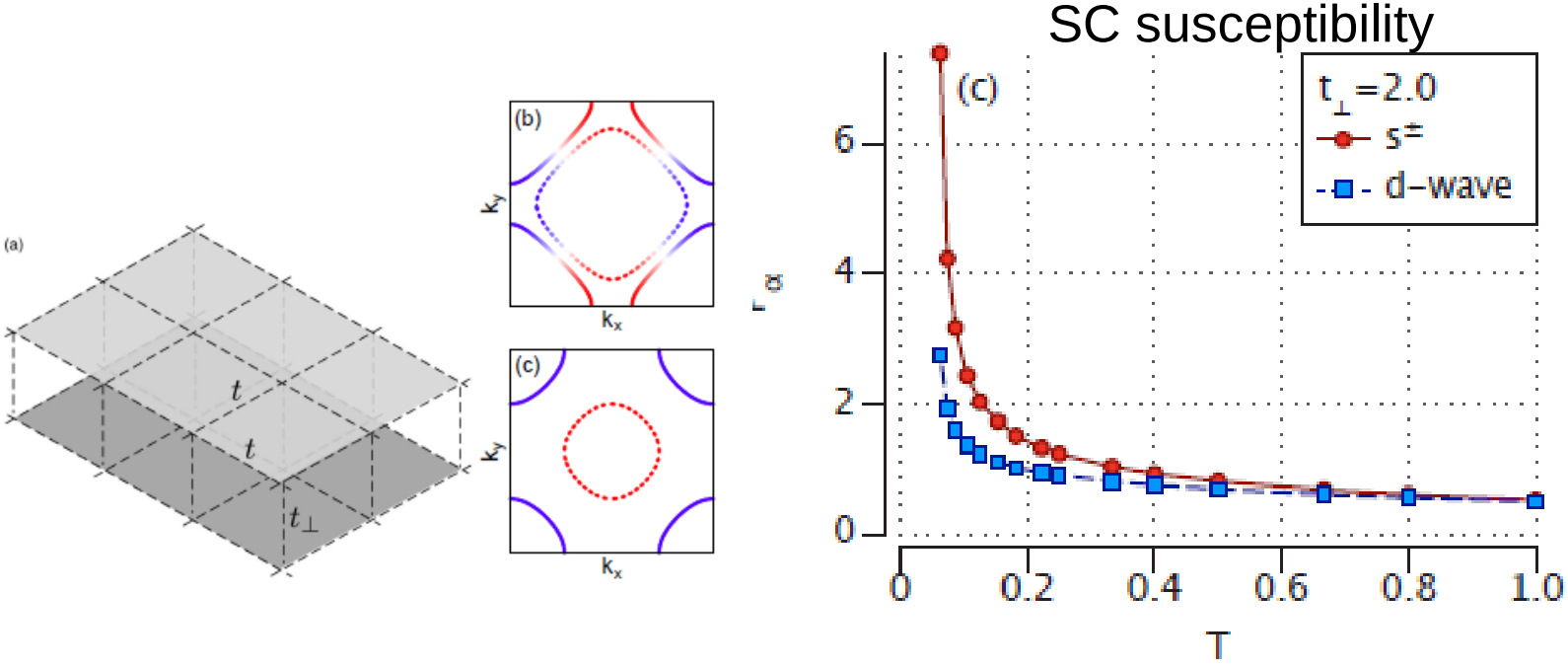




U = 8, ty = 1, tx2 = 1.2 in units of tx1

KK and R. Arita, PRB 2001,2002
Bulut et al PRB 1992
Maier & Scalapino arXiv:11070401

Dynamical Cluster Approximation



Maier & Scalapino arXiv:11070401

room temperature SC possible ??